

Power uprates
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CASL-U-2013-0196-000



Engineering design
and analysis

Demonstration of Neutronics Coupled to Thermal-Hydraulics for a Full-Core Problem using VERA

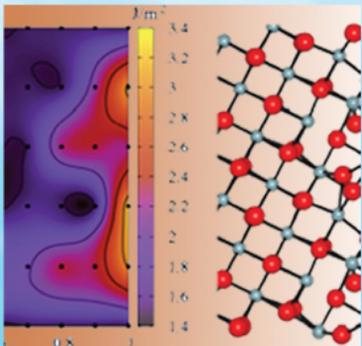
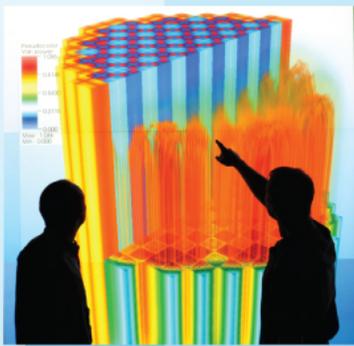
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U.S. DEPARTMENT OF
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CONTENTS

| | |
|---|-----|
| ACRONYMS | v |
| LIST OF FIGURES..... | vi |
| LIST OF TABLES..... | vii |
| 1. Introduction..... | 2 |
| Acknowledgements | 3 |
| 2. Physics Component Descriptions | 4 |
| 2.1 VERA Common Input (VERAIn) | 4 |
| 2.2 COBRA-TF (CTF) | 5 |
| 2.3 Insilico..... | 5 |
| 3. Code Coupling | 7 |
| 3.1 Introduction..... | 7 |
| 3.2 Building a Single Executable | 7 |
| 3.3 LIME | 8 |
| 3.4 Data Transfer Kit (DTK)..... | 8 |
| 3.5 Coupling Strategy | 8 |
| 4. Problem Description..... | 12 |
| 4.1 Single-Assembly Description | 12 |
| 4.2 Full-Core Description | 14 |
| 5. Single-Assembly Results | 16 |
| 5.1 Modeling Options..... | 16 |
| 5.2 Single-Assembly Results | 16 |
| 5.3 Boron Perturbations..... | 19 |
| 5.4 Power Perturbations | 22 |
| 6. Full-Core Results..... | 23 |
| 6.1 Full-Core Development..... | 23 |
| 6.2 Full-Core Modeling Options | 24 |
| 6.3 Results | 25 |
| 7. Conclusion and Recommendations..... | 31 |
| 7.1 Recommendations..... | 31 |
| 8. References..... | 33 |
| Appendix A – Property Averaging | 34 |
| A.1 Average coolant properties..... | 34 |



| | |
|---|----|
| A.2 Average fuel rod properties | 35 |
| Appendix B – Single-Assembly Input File | 37 |
| Appendix C – Full-Core Input File..... | 42 |

ACRONYMS

| | |
|--------|--|
| AMA | Advanced Modeling Applications |
| CASL | Consortium for Advanced Simulation of Light Water Reactors |
| CTF | COBRA-TF |
| DOE | U.S. Department of Energy |
| DOE-NE | U.S. Department of Energy Office of Nuclear Energy |
| DTK | Data Transfer Kit |
| FA | Focus Area |
| HFP | Hot Full Power |
| HPC | high-performance computing |
| HZP | Hot Zero Power |
| INL | Idaho National Laboratory |
| LANL | Los Alamos National Laboratory |
| LWR | light water reactor |
| MPO | Materials Performance and Optimization |
| ORNL | Oak Ridge National Laboratory |
| PCI | pellet-cladding interaction |
| PCM | percent mille (10^{-5}) |
| PNNL | Pacific Northwest National Laboratory |
| PPM | parts per million (usually boron) |
| PSU | Pennsylvania State University |
| PWR | pressurized water reactor |
| RTM | Radiation Transport Methods |
| SNL | Sandia National Laboratories |
| T-H | thermal-hydraulics |
| TPL | third-party library |
| V&V | verification and validation |
| VERA | Virtual Environment for Reactor Applications |
| VRI | Virtual Reactor Integration |

LIST OF FIGURES

| Figure | Page |
|---|-------------|
| Figure 2-1 Key components of a coupled Insilico-CTF application created to solve the example problem..... | 9 |
| Figure 2-2 Simplified flow chart illustrating the coupled code “Seidel” fixed point algorithm | 11 |
| Figure 4-1 Fuel Rod Diagram..... | 12 |
| Figure 4-2 Assembly Layout Showing Guide Tubes (GT) and Instrument Tube (IT) placement. | 13 |
| Figure 4-3 Core Layout for Watts Bar Unit 1 Cycle 1 | 15 |
| Figure 5-1 Normalized Radial Fission Rate Distribution at 600 ppm and 100% power | 17 |
| Figure 5-2 Exit Coolant Density (g/cc) at 600 ppm and 100% power | 18 |
| Figure 5-3 Axial Distributions at 600 ppm and 100% power (with fuel temperature shown)..... | 18 |
| Figure 5-4 Axial Distributions at 600 ppm and 100% power (without fuel temperature)..... | 19 |
| Figure 5-5 Axial Plot of Fission Rates at Different Boron Concentrations | 20 |
| Figure 5-6 Graphical Output of the Fission Rate, Coolant Density, and Fuel Temperatures at 0 and 1300 ppm Boron..... | 21 |
| Figure 5-7 Axial Plot of Fission Rates at Different Power Levels..... | 22 |
| Figure 6-1 2D Assembly Power Results..... | 25 |
| Figure 6-2 Axial Plots of Maximum, Minimum, and Average Rod Powers | 26 |
| Figure 6-3 3D Thermal Flux Distribution with a cutout at the top of the core | 27 |
| Figure 6-4 2D Slice of Thermal Flux Distribution near the Core Midplane | 28 |
| Figure 6-5 3D Coolant Enthalpy Distribution in the active fuel region | 29 |
| Figure 6-6 Coolant Enthalpy Distribution at the Core Exit..... | 30 |
| Figure A-1 Illustration of how a typical fuel rod is surrounded by four subchannels in a PWR square lattice fuel assembly. | 34 |
| Figure A-2 Illustrative radial discretization of a fuel rod modeled by CTF..... | 35 |

LIST OF TABLES

| Table | Page |
|--|------|
| Table 1-1 AMA Progression Benchmark Problems | 2 |
| Table 4-1 Fuel Rod and Guide Tube Descriptions | 13 |
| Table 4-2 Assembly Description | 14 |
| Table 4-3 Nominal Thermal-Hydraulic Conditions for a Single-Assembly | 14 |
| Table 4-4 Full-Core Description | 15 |
| Table 5-1 Iteration Summary at 600 ppm boron and 100% power | 17 |
| Table 5-2 Iteration Summary for Boron Cases | 19 |
| Table 5-3 Iteration Summary for Power Cases | 22 |
| Table 6-1 Iteration Summary with Restart Enabled | 25 |
| Table 6-2 Pin Power Results | 26 |

1. Introduction

This report documents the completion of Milestone L2:AMA.P7.02 – Demonstration of Neutronics Coupled to Thermal-Hydraulics for a Full-Core Problem using VERA. The purpose of this milestone is to demonstrate the modeling of a full-core PWR core with a multiphysics coupling of neutronics (including cross section and neutron transport) and thermal-hydraulics. The neutronics solution is provided by the “Insilico” code from ORNL, and the thermal-hydraulic solution is provided by the COBRA-TF (CTF) code from Penn State University (PSU). The neutronics and T/H are coupled with the LIME and DTK toolkits.

This demonstration is “Problem 7” of the AMA Progression Benchmark Problems [1]. The Progression Problems were defined to help drive development of the VERA Core Simulator capability. The progression problems serve several different functions. The first function is to help developers determine schedule and priorities for implementing features into the core simulator. This is achieved by defining a useful capability in discrete steps ranging from a single pincell up to a full-core depletion. The second function is to inform users when capabilities will be available and provide specific deliveries when users can start verification and validation studies of completed components. The third function, which was not envisioned initially, is to provide measurable metrics that management can use to gauge progress. The VERA Core Simulator is a multi-year development project and it is important to provide management with a long-term schedule and metrics to determine how well progress is being made.

The ten AMA Progression Benchmark Problems are listed in Table 1-1. The purpose of this Milestone report is to document the completion of Problem 7.

Table 1-1 AMA Progression Benchmark Problems

| |
|---|
| •#1 2D HZP Pincell |
| •#2 2D HZP Lattice |
| •#3 3D HZP Assembly |
| •#4 HZP 3x3 Assembly CRD Worth |
| •#5 Physical Reactor Zero Power Physics Tests (ZPPT) |
| •#6 HFP BOL Assembly (begin Challenge Problem coupling) |
| •#7 HFP BOC Physical Reactor w/ Xenon |
| •#8 Physical Reactor Startup Flux Maps |
| •#9 Physical Reactor Depletion |
| •#10 Physical Reactor Refueling |

Note that progression problems 1-5 are at hot zero power (HZP) conditions. At HZP, there is no sensible heat generation, and therefore, no thermal-hydraulic feedback. Problem 6 is the first progression problem that includes heat generation and requires coupled thermal-hydraulic feedback, and was documented in Milestone L3:AMA.VDT.P6.03 [2]. Problem 7 extends Problem 6 to a full-core and adds boron search capabilities.

Section 2 of this report provides a description of the computer codes used in the coupling. Section 3 provides information on how the code coupling is performed. Section 4 contains a description of the test problem used in

this Milestone. Section 5 provides results for the single assembly test cases used in Problem 6. Section 6 provides results for full-core problems used in Problem 7. Finally, Section 7 contains a conclusion, discussion of future work, and recommendations going forward.

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2. Physics Component Descriptions

This section includes descriptions of the individual physics components (CTF and Insilico) and the VERA Common Input module.

2.1 VERA Common Input (VERAIn)

The VERA Common Input (VERAIn) is a single common input used to drive all of the physics codes in the VERA Core Simulator (VERA-CS). Early in the development of the core simulator, it was recognized that it would be unreasonable to require users to generate input decks for each of the individual physics codes. This is especially true if the core simulator allows multiple codes to solve each physics problem (i.e. multiple subchannel codes, multiple neutronics solvers). In addition to the ease-of-use aspects, it is critical in multiphysics applications that all of the different code systems have consistent input. Having a single common input simplifies the user experience and helps ensure that all of the physics applications are solving a consistent geometry.

The common input is based on a single ASCII input file. The input file uses a free-form input format that is based on keyword inputs. The format of the input file was designed by engineers with broad experience with current industry core design tools, so the format of the input file will be easy for industry users to understand. The ASCII input file provides several advantages to the users:

- Allows users to easily transfer input and output between different computer systems.
- Allows users ability to easily edit the file on remote computers.
- Provides a format that users can readily read and understand.
- ASCII input files are an approved archive format recognized by the NRC (ASCII, PDF, or TIFF).
- Allows users to “diff” input files on a variety of remote computers
- Allows users to archive inputs in standard source code repositories and/or directories with read-only permissions.

The input file contains a description of the physical reactor geometry, including: fuel assemblies, removable poison assemblies, control rods, non-fuel structures, detectors, baffle, etc. The input file also contains a description of the current reactor statepoint including: power, flow, depletion, search options, etc.

In order to translate the user input to input needed for the individual code packages, a multistep process is used. First, an input parser reads the text input file and converts it into an XML file. Some physics codes, such as Insilico and MPACT, can read the XML file directly using readily-available XML libraries. Other codes, such as CTF and Peregrine, require an intermediate step that converts the XML file into the native code input. This process allows the common input file to be used for existing physics codes where we do not want to make extensive modifications to the input.

Currently, the following physics codes can interface with the VERA common input:

- Insilico
- MPACT
- COBRA-TF (CTF)
- Peregrine

Examples of VERA common input files are shown in “Appendix B – Single-Assembly Input File” and “Appendix C – Full-Core Input File”.

It should be noted that there is one class of input that cannot be readily generated by the VERA common input. Some physics codes, such as CFD, require a detailed mesh that is usually generated from a CAD file. For these codes, it is expected that the user will still have to attach an externally generated mesh file and make sure that the mesh file is consistent with the common input.

2.2 COBRA-TF (CTF)

COBRA-TF (CTF) is a thermal-hydraulic simulation code designed for Light Water Reactor (LWR) analysis [3]. CTF has a long lineage that goes back to the original COBRA program developed in 1980 by Pacific Northwest Laboratory under sponsorship of the Nuclear Regulatory Commission (NRC). The original COBRA began as a thermal-hydraulic rod-bundle analysis code, but versions of the code have been continually updated and expanded over the past several decades to cover almost all of the steady-state and transient analysis of both PWR’s and BWR’s. CTF is currently being developed and maintained by the Reactor Dynamics and Fuel Management Group (RDFMG) at the Pennsylvania State University (PSU).

CTF includes a wide range of thermal-hydraulic models important to LWR safety analysis including flow regime dependent two-phase wall heat transfer, inter-phase heat transfer and drag, droplet breakup, and quench-front tracking. CTF also includes several internal models to help facilitate the simulation of actual fuel assemblies. These models include spacer grid models, a fuel rod conduction model, and built-in material properties for both the structural materials and the coolant (i.e. steam tables).

CTF uses a two-fluid, three-field representation of the two-phase flow. The equations and fields solved are:

- Continuous vapor (mass, momentum and energy)
- Continuous liquid (mass, momentum and energy)
- Entrained liquid drops (mass and momentum)
- Non-condensable gas mixture (mass)

Some of the reasons for selecting CTF as the primary T/H solver in the VERA core simulator are the reasonable run-times compared to CFD (although CFD will be available as an option), the fact that it is being actively developed and supported by PSU, and for the ability to support future applications of VERA such as transient safety analysis and BWR and SMR applications.

2.3 Insilico

Insilico is one of the neutronics solvers in the VERA Core Simulator (along with MPACT) and is part of the Exnihilo transport suite being developed by ORNL. Insilico is the reactor toolkit package of Exnihilo and includes the reactor toolkit used for meshing of PWR geometry, and the cross section generation package based on XSPROC. Insilico uses the Denovo module [4][5] to solve for the flux and eigenvalue solutions of the 3D problem using either the discrete ordinates (S_N) solver or the Simplified Legendre (SP_N) solver. Exnihilo also includes the SHIFT Monte Carlo package, but SHIFT is not used in this study.

Multigroup cross sections are generated in Insilico using the SCALE [6]code XSProc. XSProc performs resonance self-shielding with full range Bondarenko factors using either the narrow resonance approximation or the intermediate resonance approximation. The fine energy group structure of the resonance self-shielding calculation can optionally be collapsed to a coarse group structure through a one-dimensional (1D) discrete ordinates transport calculation internal to XSProc. For all of the calculations in this study, the fine energy group structure is collapsed to either a 23-group or 11-group coarse group structure to be used in the Denovo transport solver.

The cross section libraries used in this study are the SCALE 6.2 252-group and 56-group ENDF/B-VII.0 neutron cross section libraries. These libraries contain data for 417 nuclides and 19 thermal-scattering moderators.

For coupled calculations, both the S_N and SP_N solvers have been used and tested. The S_N solver was used to generate the earlier single-assembly results and the SP_N solver was used for the larger full-core problems.

Reference [7] contains a more detailed description of the methods used in Insilico as part as the VERA Core Simulator.

3. Code Coupling

3.1 Introduction

This Milestone is a demonstration of coupling two physics codes together to calculate the temperature, fission rate, and neutron flux distribution within a PWR core. All neutronics aspects of the problem (cross-sections, neutron transport, and power release) are solved using Insilico and all thermal-hydraulic aspects (including fuel rod conduction) are solved using CTF. The coupling of these codes to create a single-executable multiphysics coupled-code application is done using the VERA infrastructure tools LIME [8] and DTK [9].

3.2 Building a Single Executable

To couple the physics codes CTF and Insilico together, both programs are combined and compiled in a single executable using the subroutine interface to CTF and Insilico along with a top-level LIME problem manager. The LIME problem manager serves as the “main” program, controls the iteration strategy, calls the CTF and Insilico subroutines as needed, and transfers data between the codes using LIME model evaluators and DTK (See Figure 2-1 below).

The single coupled executable is named “VRIPSScobra_denovo_coupled.exe” and contains all of the coupling codes. This program is located in the VERA GIT repository “PSSDrivers”:

```
PSSDriversExt/VRIPSS/drivers/cobra_denovo/VRIPSScobra_denovo_coupled.exe
```

Compiling different physics codes together can be a complicated task, especially when the packages are large and rely on additional third-party libraries (TPL’s). To overcome these complications, the TriBITS build system is used. In addition to providing the build system, TriBITS also provides an integrated testing platform to help automated developer testing.

TriBITS stands for the “Tribal Build, Integrate, and Test System” and was originally developed for Trilinos, but was later extended for VERA, SCALE and other projects. TriBITS is based on the well-known Kitware open-source toolset CMake, CTest, and CDash. Some additional features of TriBITS include the following:

- Built-in CMake-based package architecture support for partitioning a project into “Packages” with carefully regulated dependencies with numerous features including:
 - Automatic enabling of upstream and downstream packages (critical for large projects like Trilinos, SCALE, and CASL)
 - Integrated MPI and CUDA support
 - Integrated TPL support (coordinate common TPLs across unrelated packages, common behavior for user configuration, etc.)
 - Removal of a lot of boiler-plate CMake code for creating libraries, executables, copying files, etc.
- Powerful TRIBITS_ADD_[ADVANCED]_TEST(...) wrapper CMake functions to create advanced tests
- Integrated support for add-on repositories with add-on packages.
- TribitsCTestDriver.cmake testing driver:
 - Partitioned package-by-package output to CDash and reporting on a package-by-package basis
 - Failed packages don’t propagate errors to downstream packages

- Integrated coverage and memory testing (showing up on CDash)
- Nightly and continuous integration (CI) test driver.
- Pre-push synchronous CI testing with the Python checkin-test.py script
- In addition: TribitsDashboardDriver system, download-cmake.py and numerous other tools

TriBITS is an open-source project and is available for download from the internet [10].

3.3 LIME

The Lightweight Integrating Multiphysics Environment for coupling codes (LIME) is used to integrate the two physics codes [8][11]. LIME is designed to integrate separate computer codes, which may be written in different languages, into a single package to solve multiphysics problems. LIME provides high-level routines to create a “Problem Manager” to control the overall-iterations and perform communication through “Model Evaluators” for each of the separate physics codes.

A description of how LIME is used to couple CTF and Insilico is provided in Section 3.5.

LIME is an open-source project and is available for download from the internet [12].

3.4 Data Transfer Kit (DTK)

The Data Transfer Kit (DTK) library is used to transfer data between the two physics codes. DTK is based on the Rendezvous algorithm [9] and facilitates the transfer of data between multiple codes with different meshes partitioned on different parallel processors. From the DTK website:

“The Data Transfer Kit (DTK) is a software component designed to provide parallel services for mesh and geometry searching and data transfer for arbitrary physics components. In many physics applications, the concept of mesh and geometry is used to subdivide the physical domain into a discrete representation to facilitate the solution of the model problems that describe it. Additionally, the concept of the field is used to apply degrees of freedom to the mesh or geometry as a means of function discretization. With the increased development efforts in multiphysics simulation, adaptive mesh simulations, and other multiple mesh/geometry problems, generating parallel topology maps for transferring fields and other data between meshes is a common operation. DTK is being developed to provide a suite of concrete algorithm implementations for these services.”

DTK is an open-source project and is available for download from the internet [13].

3.5 Coupling Strategy

A challenging aspect of coupling neutronics and thermal-hydraulics is that the different physics associated with these two codes are strongly coupled and nonlinear. By strongly coupled we mean that the quantities calculated in each physics code and passed to the other have a significant impact on the solution of the other physics code. By nonlinear we mean that a change in values calculated in one code do NOT result in a “linearly-proportional” change to values in the other.

Figure 2-1 illustrates key aspects of the single-executable coupled-code (Insilico-CTF) simulation capability created within VERA to solve this problem.

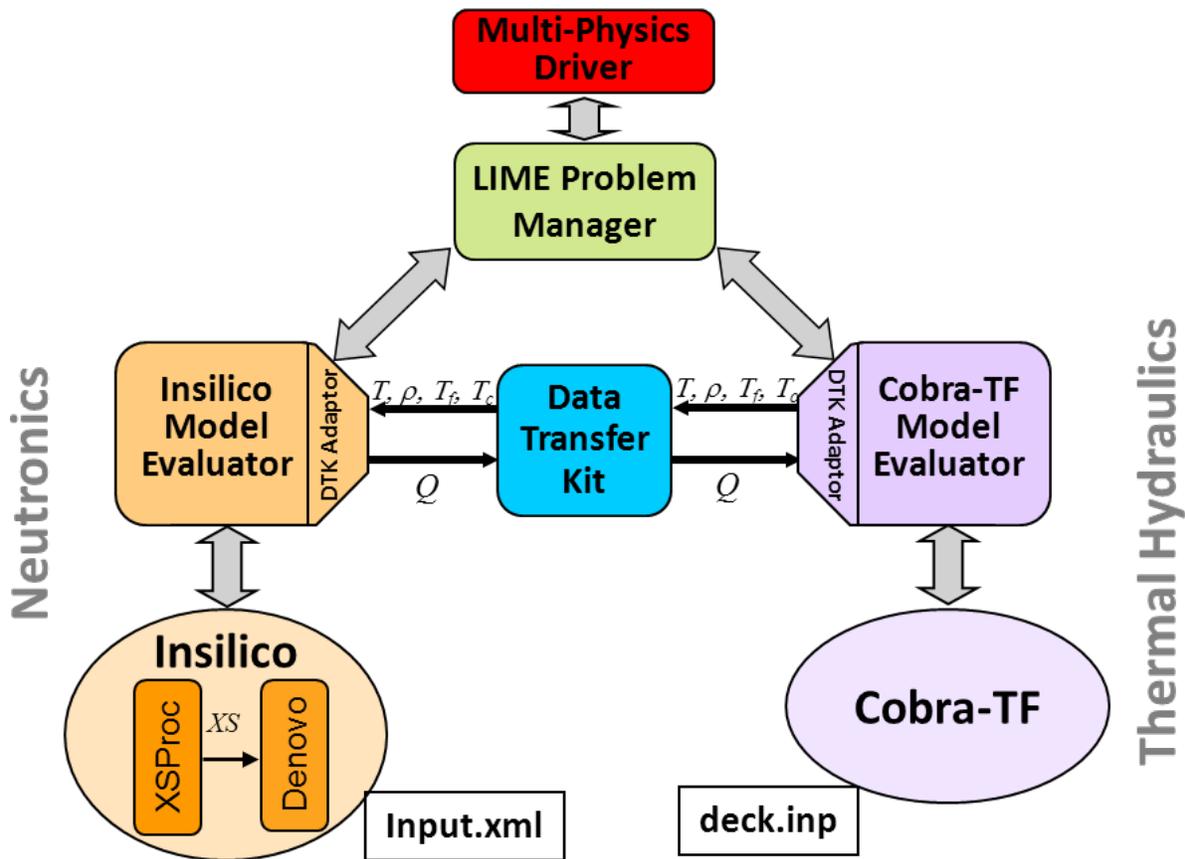


Figure 2-1 Key components of a coupled Insilico-CTF application created to solve the example problem.

To solve the neutronics part of the overall problem, Insilico must be provided with values for the following quantities associated with each rod at each axial level:

1. average fuel temperature, T_f
2. average clad temperature, T_c
3. average coolant temperature surrounding the rod, T_w
4. average coolant density surrounding the rod, ρ_w

These quantities are calculated in the CTF code and stored in the following two-dimensional arrays in the “transfer_io” module.

| | |
|--------------------|-----------------------------|
| cool_avg_den(n,jh) | Average Coolant Density |
| cool_avg_tmp(n,jh) | Average Coolant Temperature |
| clad_avg_tmp(n,jh) | Average Clad Temperature |
| fuel_avg_tmp(n,jh) | Average Fuel Temperature |

Here n denotes the fuel rod and jh the axial heat transfer level. Values in these arrays are transferred to Insilico at designated times during the overall solution procedure. Of note is that Insilico is itself solving a multiphysics neutronics problem that involves calculating cross sections, doing neutron transport, and computing energy release.

To solve the thermal hydraulics part of the problem, CTF needs the energy release rate Q in each fuel rod at each axial level. These values are computed by Insilico and transferred to CTF. Note that CTF also solves several coupled-physics equation sets internally, i.e. conservation of mass, momentum and energy in the fluid together with heat transfer to fuel rods where energy is being released and conducted within the rods.

The transfer of data between Insilico and CTF is enabled and directed by several additional software components represented in Figure 2-1 (e.g. Insilico and CTF Model Evaluators and DTK adaptors). These small components leverage LIME and DTK and provide the additional functionality needed to create the overall coupled-code simulation capability. In particular, they address the details of how and where the transfer data are stored in each code, and how to correctly transfer that data in the form required by both the “source” and the “target” during each transfer operation.

As described in references [8] and [11], LIME supports several different types of nonlinear solution strategies (i.e. Newton, Jacobian-free Newton-Krylov (JFNK), fixed point) depending on the capabilities available from the physics codes being coupled. In this case, we solve the overall coupled nonlinear system using a simple “Seidel” mode fixed point algorithm. This is an iterative method where each physics code is sequentially solved independently within a global iteration loop, and updated transfer data are passed between physics codes immediately after each physics code solution. In addition, the change in transferred values between iterations can be “relaxed” so as to improve the convergence of the approach.

The simplified execution diagram in Figure 2-2 illustrates the “Seidel” mode fixed point algorithm executed by the LIME problem manager for our example problem.

The first time CTF is asked to perform a solution, the power distribution is assumed to be uniform, unless a restart has been requested from the input. If a restart is requested, a power distribution (calculated in a previous run) is read from a restart data file. After the initial CTF solution, the power is determined by the transfer data received from the most recent Insilico calculation.

Because neither Insilico nor CTF can currently provide a residual vector to LIME, the convergence criteria used here is based on checking that key global metrics associated with the solutions in each code have reached a steady invariant condition within a user-specified tolerance. Currently the following parameters are checked for convergence:

1. Eigenvalue
2. Maximum change in local power
3. Maximum change in local fuel temperature
4. Maximum change in local clad temperature
5. Maximum change in local coolant temperature

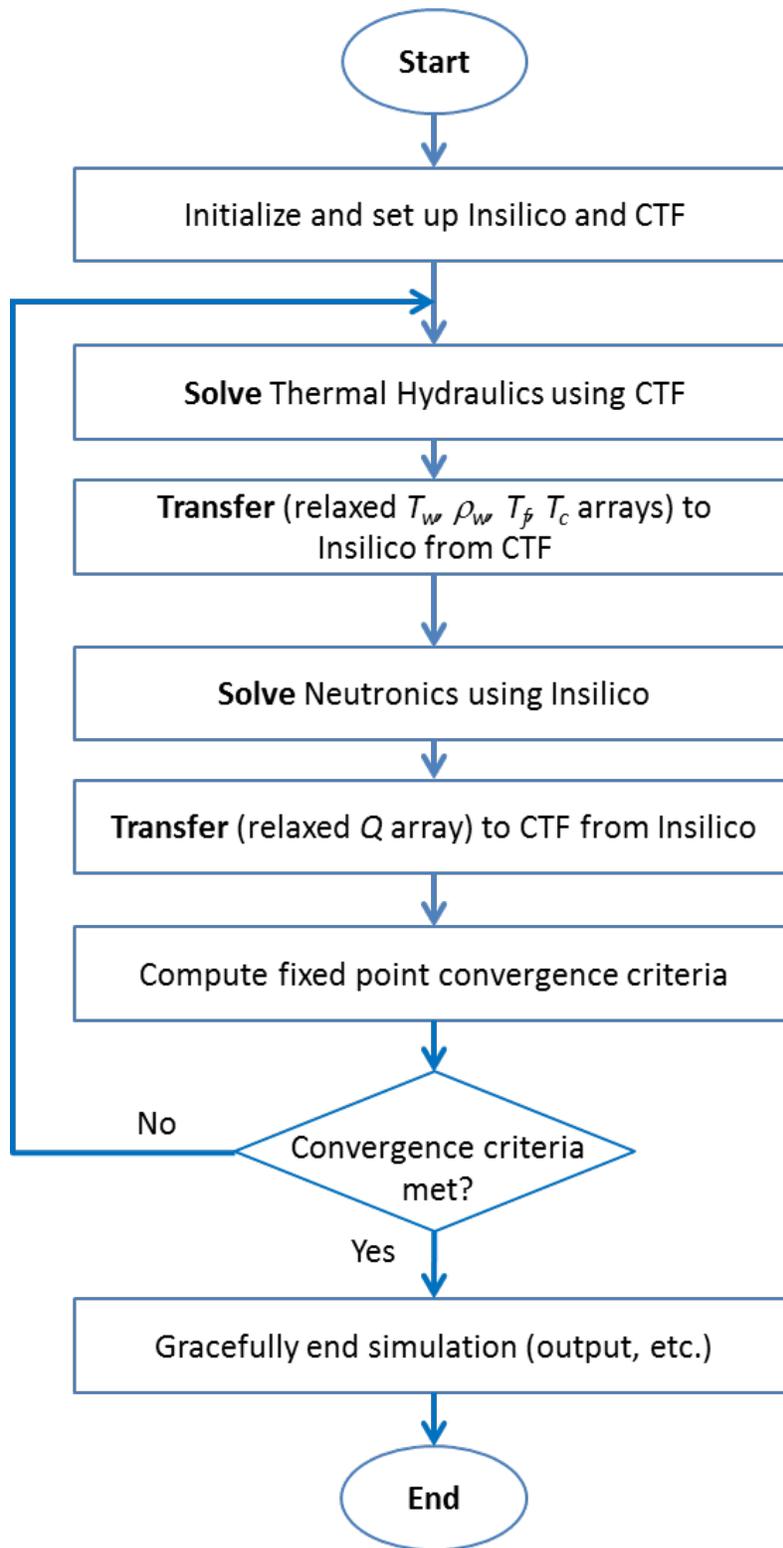


Figure 2-2 Simplified flow chart illustrating the coupled code “Seidel” fixed point algorithm

4. Problem Description

This Milestone report contains results for single-assembly and full-core calculations. The geometries are described by the AMA Progression Benchmark Problems [1] and are based on the dimensions and state conditions of Watts Bar Unit 1 Cycle 1. The single-assembly coupled problem corresponds to Problem 6, and the full-core coupled problem corresponds to Problem 7.

All dimensions are non-proprietary and are derived from the publically available Watts Bar Unit 1 FSAR [14].

4.1 Single-Assembly Description

The first example problem used in this Milestone is a PWR single assembly corresponding to AMA Progression Benchmark Problem 6. Results are shown for different boron concentrations (0, 600, and 1300 ppm) and power levels (70, 100, 130, and 150% power).

The assembly is a standard 17x17 Westinghouse fuel design with uniform fuel enrichment. There are no axial blankets or enrichment zones. The assembly has 264 fuel rods, 24 guide tubes, and a single instrument tube in the center. There are no control rods or removable burnable absorber assemblies in this problem.

The primary geometry specifications of the fuel rod and guide tube materials are given in Figure 4-1 and Table 4-1. The geometry specification for the assembly is given in Figure 4-2 and Table 4-2. For a complete description of the geometry, including spacer grid and nozzle specifications, refer to Reference [1]. The complete input listing for this problem is shown in Appendix B – Single-Assembly Input File.

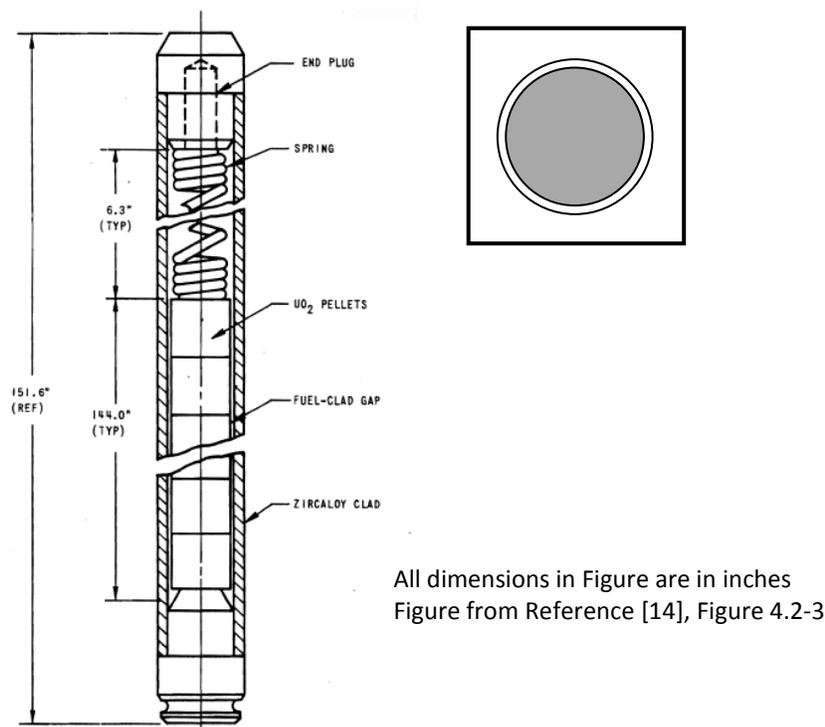


Figure 4-1 Fuel Rod Diagram

Table 4-1 Fuel Rod and Guide Tube Descriptions

| Parameter | Value | Units |
|-----------------------------------|-----------------|-------|
| Fuel Pellet Radius | 0.4096 | cm |
| Fuel Rod Clad Inner Radius | 0.418 | cm |
| Fuel Rod Clad Outer Radius | 0.475 | cm |
| Guide Tube Inner Radius | 0.561 | cm |
| Guide Tube Outer Radius | 0.602 | cm |
| Instrument Tube Inner Radius | 0.559 | cm |
| Instrument Tube Outer Radius | 0.605 | cm |
| Outside Rod Height | 385.10 | cm |
| Fuel Stack Height (active fuel) | 365.76 | cm |
| Plenum Height | 16.00 | cm |
| End Plug Heights (x2) | 1.67 | cm |
| Pellet Material | UO ₂ | |
| Clad / Caps / Guide Tube Material | Zircaloy-4 | |

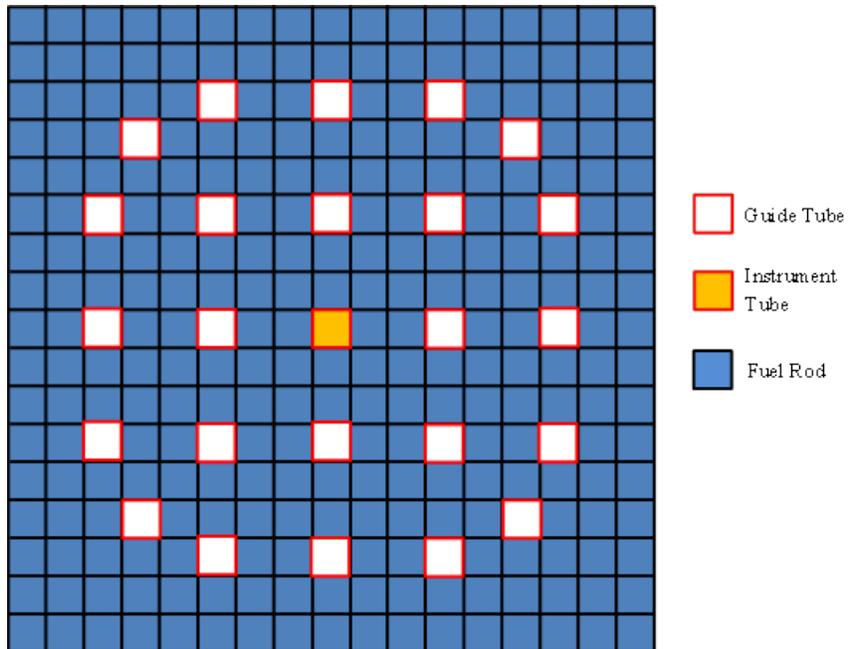


Figure 4-2 Assembly Layout Showing Guide Tubes (GT) and Instrument Tube (IT) placement.

Table 4-2 Assembly Description

| Parameter | Value | Units |
|---------------------------------|-------|-------|
| Rod Pitch | 1.26 | cm |
| Assembly Pitch | 21.5 | cm |
| Inter-Assembly Half Gaps | 0.04 | cm |
| Geometry | 17x17 | |
| Number of Fuel Rods | 264 | |
| Number of Guide Tubes (GT) | 24 | |
| Number of Instrument Tubes (IT) | 1 | |

The thermal-hydraulic specifications for this problem are shown in Table 4-3. The thermal-hydraulic conditions and feedback are what differentiate Progression Problems 3 and 6.

Table 4-3 Nominal Thermal-Hydraulic Conditions for a Single-Assembly

| Parameter | Value | Units |
|--------------------------|--------|-----------|
| Inlet Temperature | 559 | degrees F |
| System Pressure | 2250 | psia |
| Rated Flow (100% flow) | 0.6824 | Mlb/hr |
| Rated Power (100% power) | 17.67 | MWt |

4.2 Full-Core Description

The second example problem used in this Milestone is a full core PWR corresponding to AMA Progression Benchmark Problem 7. This problem corresponds to Watts Bar Unit 1 Cycle 1.

The assembly geometry descriptions for the Watts Bar core are the same as the previous section. The full-core contains 3 enrichment zones (2.1, 2.6, and 3.1% U-235) and several configurations of Pyrex burnable absorber rods. The enrichment zones and Pyrex configurations are shown in Figure 4-3. Additional Core Parameters are shown in Table 4.4. A detailed description of this reactor core is given in [7].

A partial input listing for the full-core problem is shown in Appendix C – Full-Core Input File.

| | H | G | F | E | D | C | B | A |
|----|-----------|-----------|-----------|-----------|------------------------------------|-----------|-----------|-----------|
| 8 | 2.1 | 2.6 20 | 2.1 | 2.6 20 | 2.1 | 2.6 20 | 2.1 | 3.1 12 |
| 9 | 2.6 20 | 2.1 | 2.6 24 | 2.1 | 2.6 20 | 2.1 | 3.1 24 | 3.1 |
| 10 | 2.1 | 2.6 24 | 2.1 | 2.6 20 | 2.1 | 2.6 16 | 2.1 | 3.1 8 |
| 11 | 2.6 20 | 2.1 | 2.6 20 | 2.1 | 2.6 20 | 2.1 | 3.1 16 | 3.1 |
| 12 | 2.1 | 2.6 20 | 2.1 | 2.6 20 | 2.6 | 2.6 24 | 3.1 | |
| 13 | 2.6 20 | 2.1 | 2.6 16 | 2.1 | 2.6 24 | 3.1 12 | 3.1 | |
| 14 | 2.1 | 3.1 24 | 2.1 | 3.1 16 | 3.1 | 3.1 | | |
| 15 | 3.1 12 | 3.1 | 3.1 8 | 3.1 | Enrichment Number of Pyrex Rods | | | |

Figure 4-3 Core Layout for Watts Bar Unit 1 Cycle 1

Table 4-4 Full-Core Description

| Parameter | Value | Units |
|------------------------------------|--------|-----------|
| Number of Fuel Assemblies | 193 | |
| Assembly Pitch | 21.5 | cm |
| Inlet Temperature | 559 | degrees F |
| System Pressure | 2250 | psia |
| Rated Flow (100% flow) | 131.68 | Mlb/hr |
| Rated Power (100% power) | 3411 | MWt |
| Boron Concentration | 1225 | ppm |
| Baffle Gap | 0.19 | cm |
| Baffle Thickness (stainless steel) | 2.85 | cm |

5. Single-Assembly Results

5.1 Modeling Options

All of the results in this section were run on Titan using the VERA build from 6/28/2013. Each case was run with 1156 cores (17x17 rods x 4 energy sets/decompositions).

In the neutronics solution, the Insilico S_N solver is used with the “qr” quadrature set (4 azimuthal angles and 4 polar angles per octant). The pincell calculation used 252 energy groups and is collapsed to 23 energy groups for the 3D transport solution. Insilico uses a 4x4 mesh in each fuel rod and a maximum 2.54 cm in the axial direction. Axial boundaries are positioned at each material and edit interfaces. The neutron flux is calculated from below the lower core plate to above the upper core plate in order to capture the axial leakage effects.

In the T/H solution, CTF has 49 axial levels over the active fuel region. The axial levels are defined to explicitly include the spacer grid heights, and to use uniform mesh spacing between the spacer grids. The maximum axial mesh is approximately 7 cm. The exact axial levels used in CTF are listed in the [EDITS] block of the sample input file. The CTF fuel rod heat conduction model uses 3 radial rings in each fuel rod.

Data transfer between Insilico and CTF occurs at each fuel rod on the 49 axial level mesh.

Note that these problems are not fully converged spatially in the Denovo transport solver. The purpose of this Milestone is to demonstrate the coupling between neutronics and T/H, so a somewhat coarse spatial discretization is used in Denovo to reduce problem run-times. One recommendation for future work is to determine the set of input parameters needed to converge the transport problem in spatial mesh, angle, scattering angle, and energy. (See further recommendations in Section 7.1.)

5.2 Single-Assembly Results

A typical iteration summary for the single-assembly at 600 ppm boron is shown in Table 5-1.

- The first column shows the coupled iteration count.
- The second column (its) shows the number of Denovo iterations taken per coupled iteration.
- The third column (xkeff) shows the reactor eigenvalue.
- The fourth column (keff_dif) shows the change in eigenvalue between coupled iterations.
- The fifth column (powr_dif) shows the change in local power between coupled iterations.
- The sixth column shows the maximum coolant temperature (degrees F, which are native CTF units) averaged over a single subchannel mesh and axial mesh.
- The seventh and eighth columns show the maximum clad and fuel temperatures (degrees F, which are native CTF units) averaged over a single fuel rod and axial mesh.
- The ninth through eleventh columns show the change in peak temperatures between iterations for the coolant, clad, and fuel respectively.

Table 5-1 Iteration Summary at 600 ppm boron and 100% power

| its | xkeff | keff_dif | powr_dif | cool temp | clad temp | fuel temp | cool delta | clad delta | fuel delta | |
|-----|-------|------------|----------|-----------|-----------|-----------|------------|------------|------------|---------|
| 1 | 27 | 1.23376105 | 18947.0 | 1.000000 | 623.60 | 705.40 | 2109.00 | 64.55 | 128.00 | 1218.00 |
| 2 | 22 | 1.23302139 | 60.0 | 0.222356 | 623.58 | 698.42 | 2038.82 | 0.03 | -7.00 | -69.94 |
| 3 | 19 | 1.23336920 | 28.2 | 0.040185 | 623.70 | 697.68 | 2003.28 | 0.12 | -0.74 | -35.53 |
| 4 | 15 | 1.23339591 | 2.2 | 0.004610 | 623.61 | 698.01 | 2013.56 | -0.09 | 0.33 | 10.28 |
| 5 | 9 | 1.23341182 | 1.3 | 0.000644 | 623.57 | 698.32 | 2018.20 | -0.04 | 0.31 | 4.64 |
| 6 | 5 | 1.23343045 | 1.5 | 0.000166 | 623.69 | 698.45 | 2021.05 | 0.12 | 0.12 | 2.85 |
| 7 | 2 | 1.23344063 | 0.8 | 0.000015 | 623.68 | 698.54 | 2022.51 | -0.02 | 0.10 | 1.46 |
| 8 | 1 | 1.23343920 | 0.1 | 0.000000 | 623.67 | 698.59 | 2023.22 | -0.01 | 0.05 | 0.71 |
| 9 | 1 | 1.23343781 | 0.1 | 0.000000 | 623.66 | 698.62 | 2023.59 | -0.01 | 0.03 | 0.37 |
| 10 | 1 | 1.23343668 | 0.1 | 0.000000 | 623.66 | 698.63 | 2023.77 | -0.00 | 0.01 | 0.18 |
| 11 | 1 | 1.23343567 | 0.1 | 0.000000 | 623.66 | 698.64 | 2023.87 | -0.00 | 0.01 | 0.10 |

Note that the convergence criterion for this problem is very tight. The eigenvalue convergence is set to 5 pcm (5×10^{-5} delta-k). The most limiting convergence criteria is the maximum change in peak fuel temperature, which has a convergence criteria of 0.1 degrees F. All of the coupled iteration parameters are set in the [COUPLED] block of the input file.

The normalized radial fission rate distribution integrated over the axial direction is shown in Figure 5-1. Note that the results are octant symmetric and there is no power in the guide tubes or instrument tubes.

| | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0.939 | 0.932 | 0.936 | 0.947 | 0.958 | 0.968 | 0.966 | 0.966 | 0.970 | 0.966 | 0.966 | 0.968 | 0.958 | 0.947 | 0.936 | 0.932 | 0.939 |
| 0.932 | 0.928 | 0.939 | 0.958 | 0.981 | 1.014 | 0.986 | 0.986 | 1.013 | 0.986 | 0.986 | 1.014 | 0.981 | 0.958 | 0.939 | 0.928 | 0.932 |
| 0.936 | 0.939 | 0.970 | 1.022 | 1.046 | | 1.033 | 1.031 | | 1.031 | 1.033 | | 1.046 | 1.022 | 0.970 | 0.939 | 0.936 |
| 0.947 | 0.958 | 1.022 | | 1.064 | 1.054 | 1.011 | 1.007 | 1.037 | 1.007 | 1.011 | 1.054 | 1.064 | | 1.022 | 0.958 | 0.947 |
| 0.958 | 0.981 | 1.046 | 1.064 | 1.041 | 1.054 | 1.013 | 1.010 | 1.041 | 1.010 | 1.013 | 1.054 | 1.041 | 1.064 | 1.046 | 0.981 | 0.958 |
| 0.968 | 1.014 | | 1.054 | 1.054 | | 1.044 | 1.042 | | 1.042 | 1.044 | | 1.054 | 1.054 | | 1.014 | 0.968 |
| 0.966 | 0.986 | 1.033 | 1.011 | 1.013 | 1.044 | 1.011 | 1.011 | 1.042 | 1.011 | 1.011 | 1.044 | 1.013 | 1.011 | 1.033 | 0.986 | 0.966 |
| 0.966 | 0.986 | 1.031 | 1.007 | 1.010 | 1.042 | 1.011 | 1.010 | 1.042 | 1.010 | 1.011 | 1.042 | 1.010 | 1.007 | 1.031 | 0.986 | 0.966 |
| 0.970 | 1.013 | | 1.037 | 1.041 | | 1.042 | 1.042 | | 1.042 | 1.042 | | 1.041 | 1.037 | | 1.013 | 0.970 |
| 0.966 | 0.986 | 1.031 | 1.007 | 1.010 | 1.042 | 1.011 | 1.010 | 1.042 | 1.010 | 1.011 | 1.042 | 1.010 | 1.007 | 1.031 | 0.986 | 0.966 |
| 0.966 | 0.986 | 1.033 | 1.011 | 1.013 | 1.044 | 1.011 | 1.011 | 1.042 | 1.011 | 1.011 | 1.044 | 1.013 | 1.011 | 1.033 | 0.986 | 0.966 |
| 0.968 | 1.014 | | 1.054 | 1.054 | | 1.044 | 1.042 | | 1.042 | 1.044 | | 1.054 | 1.054 | | 1.014 | 0.968 |
| 0.958 | 0.981 | 1.046 | 1.064 | 1.041 | 1.054 | 1.013 | 1.010 | 1.041 | 1.010 | 1.013 | 1.054 | 1.041 | 1.064 | 1.046 | 0.981 | 0.958 |
| 0.947 | 0.958 | 1.022 | | 1.064 | 1.054 | 1.011 | 1.007 | 1.037 | 1.007 | 1.011 | 1.054 | 1.064 | | 1.022 | 0.958 | 0.947 |
| 0.936 | 0.939 | 0.970 | 1.022 | 1.046 | | 1.033 | 1.031 | | 1.031 | 1.033 | | 1.046 | 1.022 | 0.970 | 0.939 | 0.936 |
| 0.932 | 0.928 | 0.939 | 0.958 | 0.981 | 1.014 | 0.986 | 0.986 | 1.013 | 0.986 | 0.986 | 1.014 | 0.981 | 0.958 | 0.939 | 0.928 | 0.932 |
| 0.939 | 0.932 | 0.936 | 0.947 | 0.958 | 0.968 | 0.966 | 0.966 | 0.970 | 0.966 | 0.966 | 0.968 | 0.958 | 0.947 | 0.936 | 0.932 | 0.939 |

Figure 5-1 Normalized Radial Fission Rate Distribution at 600 ppm and 100% power

A map of the coolant density in the top axial elevation of the core is shown in Figure 5-2. The coolant density shown in this map is the average density surrounding each rod, not the density in each CTF channel. The calculation for this density is described in Appendix A – Property Averaging. Note that the exit density is lower in the center of the assembly, corresponding to the higher fuel rod powers shown in Figure 5-1.

Average axial distributions for this problem are shown in Figures 5-3 and 5-4. Figure 5-3 includes the fuel temperature and Figure 5-4 does not include the fuel temperature so the coolant and clad temperature profiles are easier to see.

Note the small “dips” in the axial fission rate and fuel temperature profiles. These dips are due to the presence of spacer grids. The spacer grids displace moderator in the coolant channels and decrease the neutron moderation around the grids. The decreased moderation causes a local depression in the flux and power.

| | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0.659 | 0.658 | 0.657 | 0.656 | 0.656 | 0.655 | 0.655 | 0.655 | 0.655 | 0.655 | 0.655 | 0.655 | 0.656 | 0.656 | 0.657 | 0.658 | 0.659 |
| 0.658 | 0.657 | 0.657 | 0.656 | 0.655 | 0.655 | 0.654 | 0.654 | 0.654 | 0.654 | 0.654 | 0.655 | 0.655 | 0.656 | 0.657 | 0.657 | 0.658 |
| 0.657 | 0.657 | 0.656 | 0.655 | 0.654 | 0.654 | 0.653 | 0.653 | 0.653 | 0.653 | 0.653 | 0.654 | 0.654 | 0.655 | 0.656 | 0.657 | 0.657 |
| 0.656 | 0.656 | 0.655 | 0.654 | 0.653 | 0.653 | 0.652 | 0.652 | 0.652 | 0.652 | 0.652 | 0.652 | 0.653 | 0.653 | 0.654 | 0.655 | 0.656 |
| 0.656 | 0.655 | 0.654 | 0.653 | 0.653 | 0.652 | 0.652 | 0.652 | 0.652 | 0.652 | 0.652 | 0.652 | 0.652 | 0.653 | 0.653 | 0.654 | 0.655 |
| 0.655 | 0.655 | 0.654 | 0.653 | 0.652 | 0.652 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.652 | 0.652 | 0.653 | 0.654 | 0.655 |
| 0.655 | 0.654 | 0.653 | 0.652 | 0.652 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.652 | 0.652 | 0.653 | 0.654 |
| 0.655 | 0.654 | 0.653 | 0.652 | 0.652 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.652 | 0.652 | 0.653 | 0.654 |
| 0.655 | 0.654 | 0.653 | 0.652 | 0.652 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.652 | 0.652 | 0.653 | 0.654 |
| 0.655 | 0.654 | 0.653 | 0.652 | 0.652 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.652 | 0.652 | 0.653 | 0.654 |
| 0.655 | 0.654 | 0.653 | 0.652 | 0.652 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.652 | 0.652 | 0.653 | 0.654 |
| 0.655 | 0.655 | 0.654 | 0.653 | 0.652 | 0.652 | 0.651 | 0.651 | 0.651 | 0.651 | 0.651 | 0.652 | 0.652 | 0.653 | 0.654 | 0.655 | 0.655 |
| 0.656 | 0.655 | 0.654 | 0.653 | 0.653 | 0.652 | 0.652 | 0.652 | 0.652 | 0.652 | 0.652 | 0.652 | 0.653 | 0.653 | 0.654 | 0.655 | 0.656 |
| 0.656 | 0.656 | 0.655 | 0.654 | 0.653 | 0.653 | 0.652 | 0.652 | 0.652 | 0.652 | 0.652 | 0.652 | 0.653 | 0.653 | 0.654 | 0.655 | 0.656 |
| 0.657 | 0.657 | 0.656 | 0.655 | 0.654 | 0.654 | 0.653 | 0.653 | 0.653 | 0.653 | 0.653 | 0.654 | 0.654 | 0.655 | 0.656 | 0.657 | 0.657 |
| 0.658 | 0.657 | 0.657 | 0.656 | 0.655 | 0.655 | 0.654 | 0.654 | 0.654 | 0.654 | 0.654 | 0.655 | 0.655 | 0.656 | 0.657 | 0.657 | 0.658 |
| 0.659 | 0.658 | 0.657 | 0.656 | 0.656 | 0.655 | 0.655 | 0.655 | 0.655 | 0.655 | 0.655 | 0.655 | 0.656 | 0.656 | 0.657 | 0.658 | 0.659 |

Figure 5-2 Exit Coolant Density (g/cc) at 600 ppm and 100% power

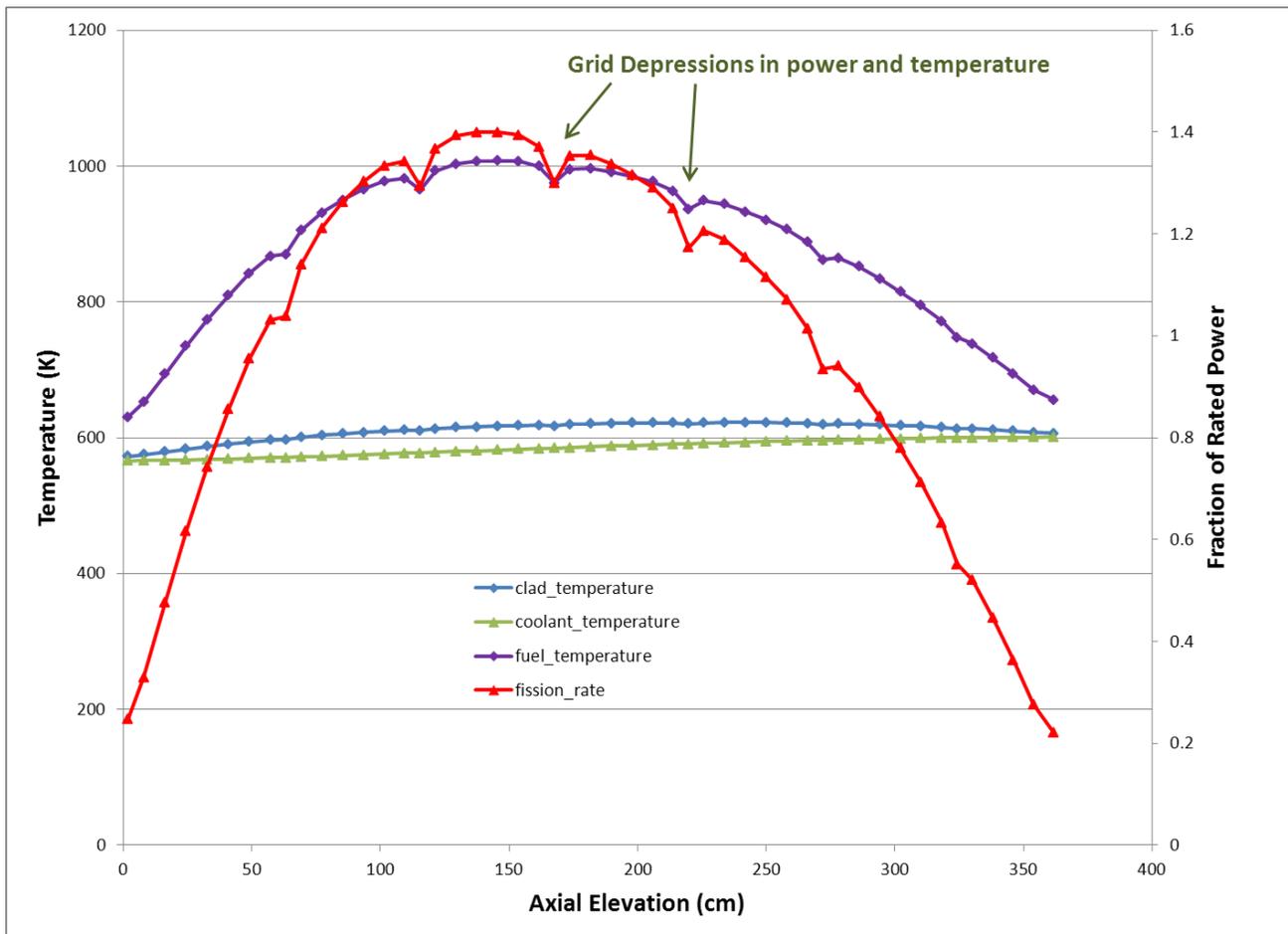


Figure 5-3 Axial Distributions at 600 ppm and 100% power (with fuel temperature shown)

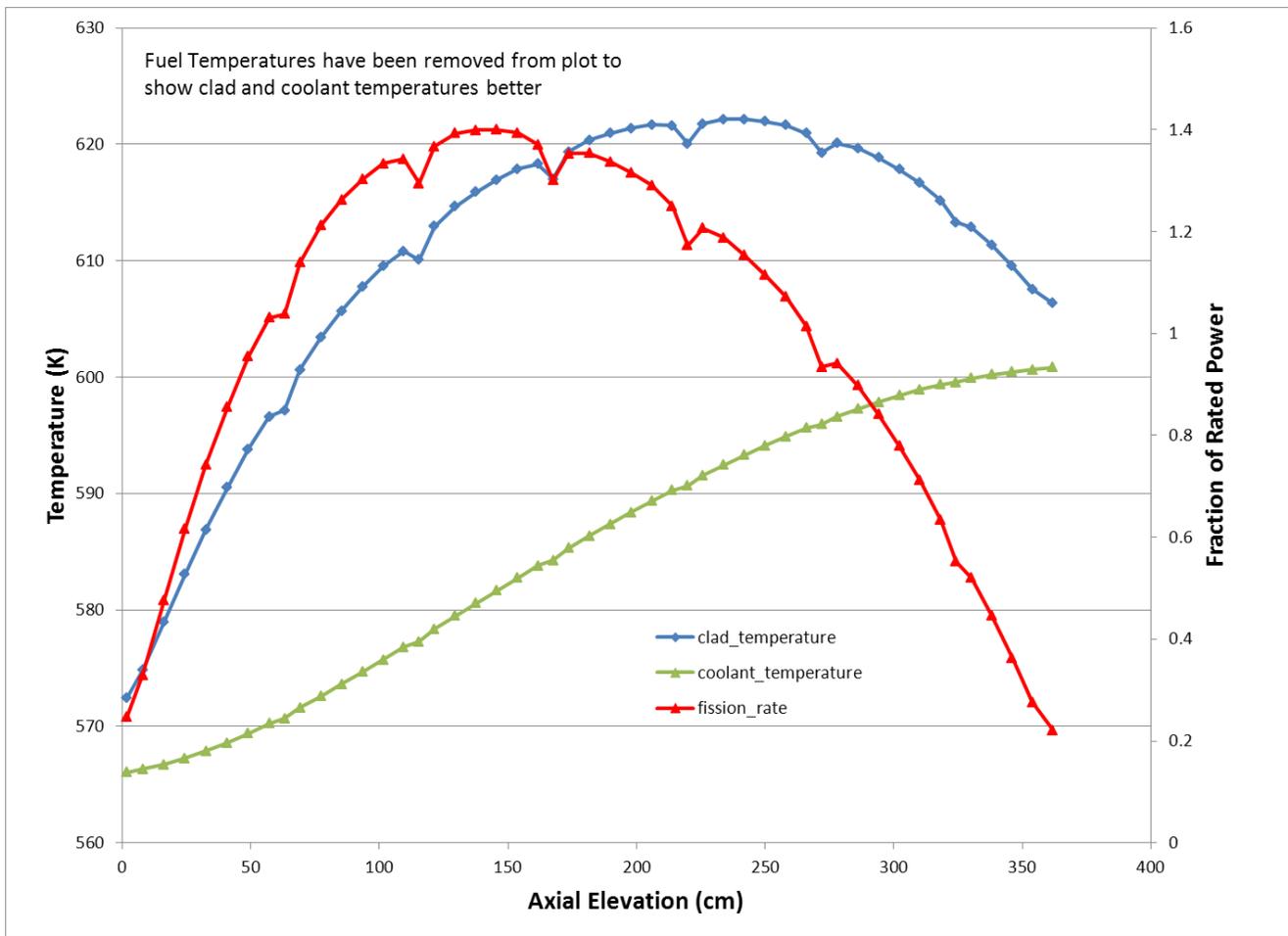


Figure 5-4 Axial Distributions at 600 ppm and 100% power (without fuel temperature)

5.3 Boron Perturbations

In order to see the effects of different boron concentrations on the results, the single-assembly case was run at three different boron concentrations – 0, 600, and 1300 ppm boron. The eigenvalues and wall-clock times for these cases are listed in Table 5-2.

Table 5-2 Iteration Summary for Boron Cases

| Boron Concentration | Eigenvalue | Wall Time (HH:MM:SS) | Coupled Iterations |
|---------------------|------------|----------------------|--------------------|
| 0 ppm | 1.31286 | 5:11:54 | 11 |
| 600 ppm | 1.23344 | 4:27:23 | 11 |
| 1300 ppm | 1.15336 | 4:06:21 | 11 |

The fission rate and fuel temperature profiles for three different boron concentrations are shown in Figure 5-5. With T/H feedback, the fission rate shape is shifted lower in the core from the normal cosine-shaped distribution you would see with no T/H feedback. The reason for this downward shift in the fission rate is that the coolant density is higher at the bottom of the core, and the higher coolant density increases the neutron moderation. As

more boron is added, the additional neutron absorption counters the higher moderation, and less power shift towards the bottom of the core is observed.

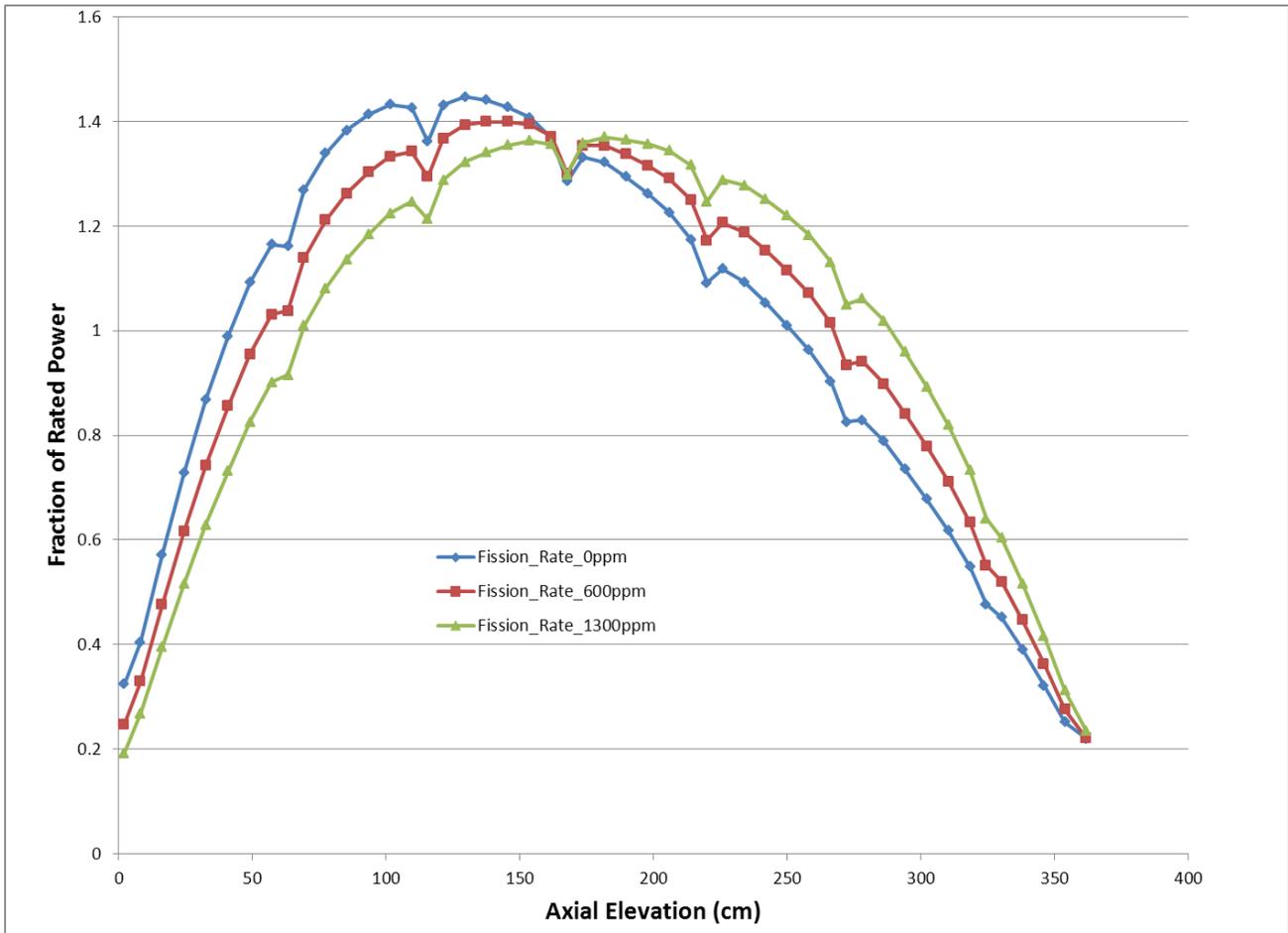


Figure 5-5 Axial Plot of Fission Rates at Different Boron Concentrations

In order to look at 3D distributions, the coupled code also produces output in the form of SILO files. These files can be used by visualization tools, such as VisIt or ParaView, to look at 3D plots of the output. Figure 5-6 shows an example of 3D distributions of the fission rate, coolant density, and fuel temperature for cases at 0 ppm and 1300 ppm boron. (Note that the results in this figure were generated with different code options and are not consistent with the results in the other figures.)

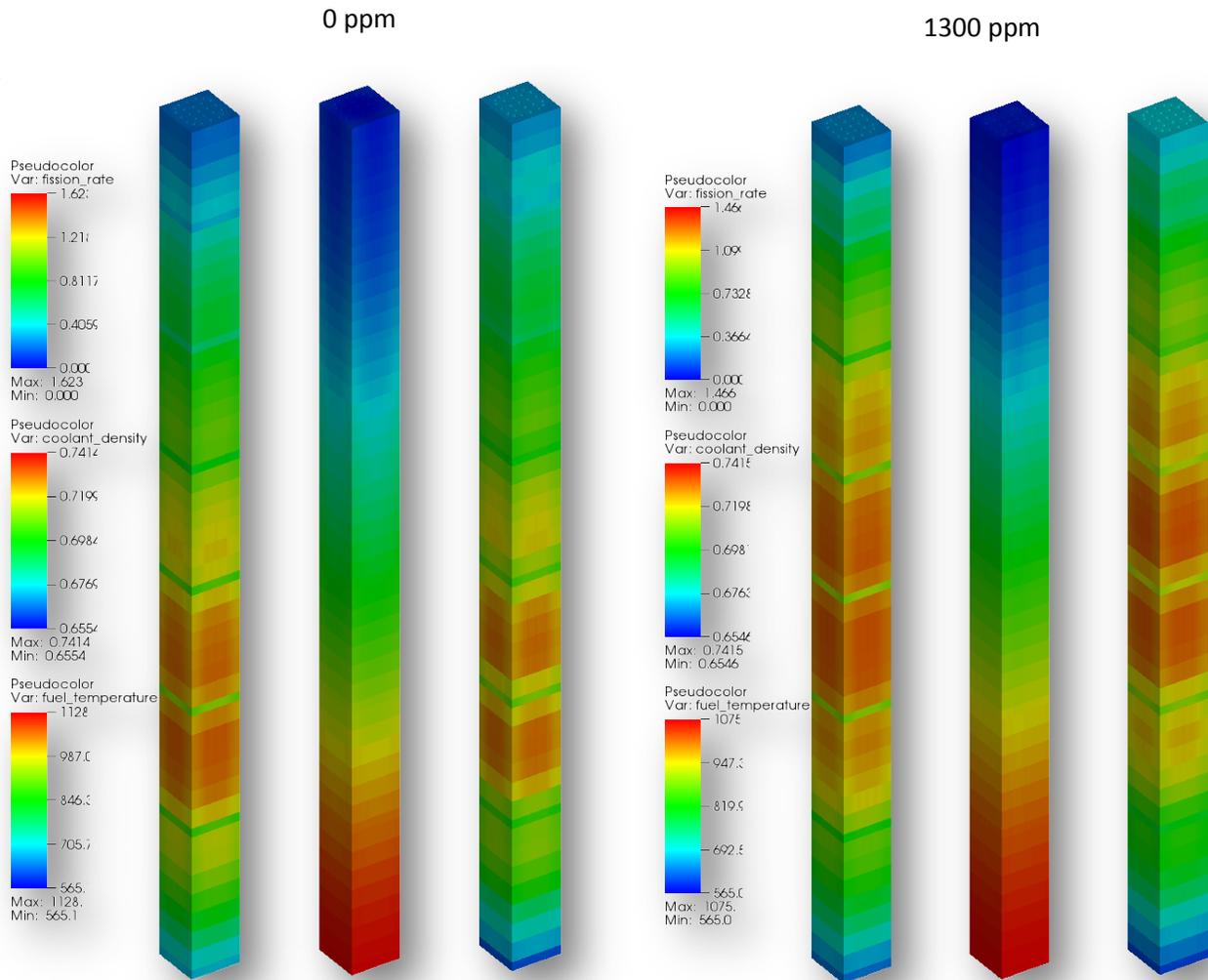


Figure 5-6 Graphical Output of the Fission Rate, Coolant Density, and Fuel Temperatures at 0 and 1300 ppm Boron

5.4 Power Perturbations

In order to see the effects of different power levels on the results, the nominal single-assembly case was run at three different power levels – 70, 100, and 130% power. The eigenvalues and wall-clock times for these cases are shown in Table 5-3.

Table 5-3 Iteration Summary for Power Cases

| Power Level | Eigenvalue | Wall Time (HH:MM:SS) | Coupled Iterations |
|-------------|------------|----------------------|--------------------|
| 70% | 1.24012 | 4:39:20 | 11 |
| 100% | 1.23344 | 4:27:23 | 11 |
| 130% | 1.22643 | 6:22:01 | 15 |

The fission rate profiles for the four power cases are shown in Figure 5-7. At higher power levels, the fission rate shape is shifted lower in the core from the normal cosine-shaped distribution you would see with no T/H feedback.

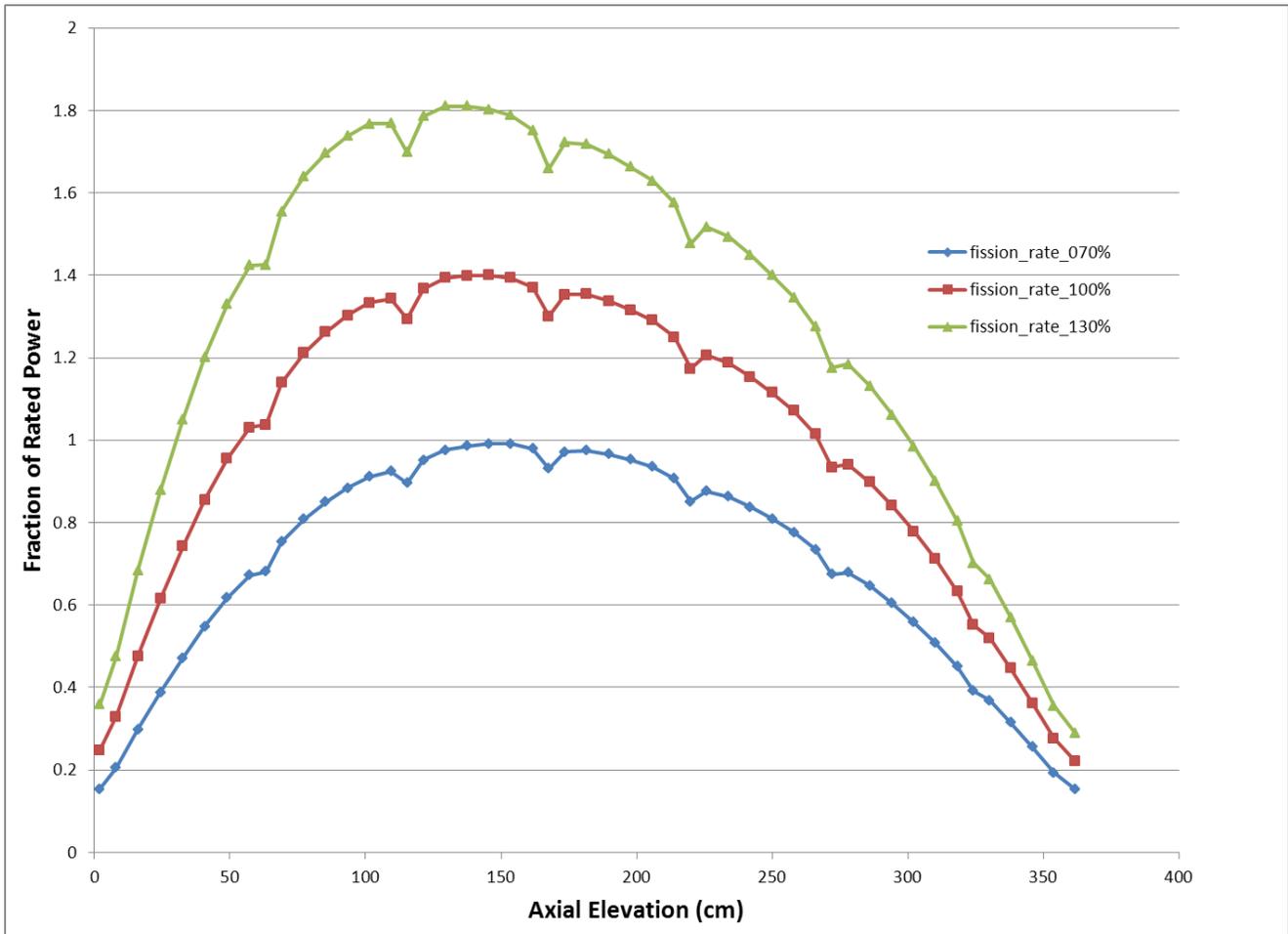


Figure 5-7 Axial Plot of Fission Rates at Different Power Levels

6. Full-Core Results

This section contains results for a full-core model run with a coupled Insilico-CTF solver using quarter-core symmetry.

6.1 Full-Core Development

Several obstacles were encountered and overcome when scaling the coupled solution from a single-assembly calculation to a full-core calculation. These included:

1. Scaling geometry from single-assembly to full-core

In the initial implementation of the cross section processing and meshing, the entire problem geometry was stored in memory on a single processor. This worked for smaller problems, but as the size of the problem grew, the geometry and cross section information for the entire problem would no longer fit on a single processor. The cross section and geometry processing had to be re-factored to split the core geometry onto multiple processors.

2. Scaling unique regions from single-assembly to full-core

In a coupled calculation, each fuel rod and each axial elevation has a unique temperature and density for the moderator and fuel, and will therefore have a unique set of cross sections for that region. For the full-core problem, the number of unique regions is calculated by:

- 15 assemblies across the problem
- 17 rods across each assembly
- 20 regions across in the radial reflector/baffle
- 49 axial levels in the fuel
- additional axial levels for the nozzle, core plate, and axial reflector

for a total of 3,705,625 unique regions, not including the additional axial regions. For quarter-core symmetry, this number drops to 933,156 regions. Additional development and code-refactoring had to be performed to distribute the number of cross section sets for the unique regions over multiple processors.

3. Scaling of CTF to run full-core geometries

When running a single-assembly calculation in CTF, the run-times are on the order of several minutes when run in serial. For full-core problems, the CTF run-times grow dramatically and take over 25 hours to run a single CTF calculation in serial. This run-time was unacceptable for coupled solutions and CTF was modified to run in parallel. In a parallel CTF calculation, the CTF run-time for a full-core problem has been reduced to less than 10 minutes per statepoint.

Additional information on the parallel CTF efforts can be found in Milestone L3:VRI.PSS.P7.05 [15].

4. Search for critical boron concentration

One requirement for this Milestone was to add a boron search option. This capability has been completed and successfully tested. Coupled problems can now be run with either an eigenvalue search or a critical boron search.

5. Run-times exceed queue run-time limits

The full-core problems require many more parallel processors than single-assembly calculations. The larger jobs lead to longer queue-times in batch processing systems (like Titan), and the jobs may not even finish in the maximum run-times allowed by the batch systems. To overcome the maximum run-times and reduce the number of jobs required, a “restart” capability was implemented to restart a calculation from a power distribution calculated from a previous calculation. This allowed long-running jobs to be completed using multiple job submissions.

6. Model additional full-core features (reflectors/baffles)

The full-core problem required the additional of a “ragged” core geometry in the radial direction and the addition of a radial reflector and steel reflector surrounding the core. These geometry features can be observed in the figures below.

6.2 Full-Core Modeling Options

This section describes the modeling options used to model the full-core reactor. The full-core results were run with a VERA build from 12/17/2013. The results were run on Titan using 18,769 cores (137x137).

The neutronics solution was generated with Insilico using cross sections from XSPROC and the SP_N 3D transport solver. XSPROC generates cross sections for each unique region by running a 56-group pincell calculation (BONAMI and XSDRN) for each region and spatially averaging the cross sections over the fuel rod and collapsing to 11 energy groups for the 3D transport solve. The 3D SP_N solver uses a SP_3 solution with P1 scattering, a 2x2 mesh in each fuel rod, and a maximum axial mesh of 2.54 cm. Axial boundaries are positioned at each material and coupling interface. The neutron flux is calculated from below the lower core plate to above the upper core plate in order to capture the axial leakage effects.

The T/H solution is generated with CTF using 49 axial levels in the active fuel region. The axial levels are defined to explicitly include the spacer grid heights, and to use uniform mesh spacing between the spacer grids. The maximum axial mesh is approximately 7 cm. The exact axial levels used in CTF are listed in the [EDITS] block of the sample input file. The CTF fuel rod heat conduction model uses 3 radial rings in each fuel rod.

Data transfer between Insilico and CTF occurs at each fuel rod on the 49 axial level mesh (the “coupling mesh”).

Note that the Insilico transport solver may not be fully converged spatially. The purpose of this Milestone is to demonstrate the coupling between neutronics and T/H. We believe the mesh is close to convergence, but no mesh studies have been performed to confirm this. One recommendation for future work is to determine the set of input parameters needed to converge the transport solver in spatial mesh, angle, scattering angle, and energy. (See further recommendations in Section 7.1.)

6.3 Results

The iteration summary for the full-core calculation is shown in Table 6-1. This calculation was performed in two separate runs on Titan. The first run took 7 iterations before hitting the run-time limit of 12:00 hours on Titan. The second run was restarted from the power calculated in the first run and took an additional 3 iterations. The total run took 10 iterations and approximately 17.5 hours.

Definitions for each of the columns of Table 6-1 are given at the top of Section 5.2.

Table 6-1 Iteration Summary with Restart Enabled

| | its | xkeff | keff_dif | powr_dif | cool | clad | fuel | delta | delta | delta |
|---|------|----------|----------|----------|--------|--------|---------|-------|--------|---------|
| 1 | 1247 | 0.986477 | -1352.3 | 1.000000 | 622.00 | 693.70 | 1525.00 | 64.62 | 95.07 | 127.20 |
| 2 | 1042 | 0.984064 | -241.3 | 0.065975 | 634.42 | 723.89 | 2399.87 | 12.47 | 30.16 | 875.10 |
| 3 | 908 | 0.983410 | -65.4 | 0.012352 | 638.80 | 735.91 | 2649.67 | 4.38 | 12.02 | 249.80 |
| 4 | 351 | 0.983204 | -20.6 | 0.002382 | 639.75 | 738.99 | 2717.49 | 0.95 | 3.08 | 67.82 |
| 5 | 569 | 0.983137 | -6.7 | 0.001741 | 640.00 | 739.73 | 2738.42 | 0.25 | 0.74 | 20.93 |
| 6 | 502 | 0.983113 | -2.4 | 0.000622 | 640.18 | 740.06 | 2744.71 | 0.18 | 0.33 | 6.29 |
| 7 | 152 | 0.983103 | -1.0 | 0.000081 | 640.26 | 740.19 | 2746.94 | 0.08 | 0.12 | 2.23 |
| Start date: Thu Dec 19 23:29:56 EST 2013 | | | | | | | | | | |
| End date: (job stopped after 12:00 hours) | | | | | | | | | | |
| | its | xkeff | keff_dif | powr_dif | cool | clad | fuel | delta | delta | delta |
| 1 | 1443 | 0.983100 | -1690.0 | 0.000668 | 640.90 | 740.40 | 2748.00 | 83.62 | 141.70 | 1350.00 |
| 2 | 241 | 0.983101 | 0.1 | 0.000419 | 640.97 | 740.35 | 2747.97 | 0.01 | 0.01 | -0.51 |
| 3 | 10 | 0.983100 | -0.1 | 0.000002 | 640.97 | 740.35 | 2748.07 | 0.00 | -0.00 | 0.10 |
| Start date: Fri Dec 20 18:08:37 EST 2013 | | | | | | | | | | |
| End date: Fri Dec 20 23:40:50 EST 2013 | | | | | | | | | | |
| elapsed time 5:32:13 332.22 min | | | | | | | | | | |

The large number of neutronic iterations in the “its” column is an artifact of the Davidson eigenvalue method used by the SP_N solver, which effectively combines the inner and outer iterations into a single iteration count.

The 2D assembly power results (axially integrated and assembly averaged) are shown in Figure 6-1. The maximum relative assembly power is 1.2758 and the minimum relative assembly power is 0.6337, which occurs on the core boundary.

The minimum and maximum pin power results are shown in Table 6-2. A plot of the maximum, minimum, and average axial rod powers is shown in Figure 6-2.

| | H | G | F | E | D | C | B | A |
|----|--------|--------|--------|--------|--------|--------|--------|--------|
| 8 | 1.0619 | 0.9815 | 1.0605 | 1.0222 | 1.1330 | 1.0491 | 1.0550 | 0.7740 |
| 9 | 0.9815 | 1.0500 | 0.9428 | 1.1053 | 1.0612 | 1.1452 | 1.0334 | 0.8806 |
| 10 | 1.0605 | 0.9428 | 1.0856 | 1.0489 | 1.1641 | 1.1257 | 1.0682 | 0.7859 |
| 11 | 1.0222 | 1.1053 | 1.0489 | 1.1592 | 1.0830 | 1.1298 | 1.0218 | 0.6516 |
| 12 | 1.1330 | 1.0612 | 1.1641 | 1.0830 | 1.2758 | 0.8979 | 0.9334 | |
| 13 | 1.0491 | 1.1452 | 1.1257 | 1.1298 | 0.8979 | 0.9134 | 0.6337 | |
| 14 | 1.0550 | 1.0334 | 1.0682 | 1.0218 | 0.9334 | 0.6337 | | |
| 15 | 0.7740 | 0.8806 | 0.7859 | 0.6516 | | | | |

Figure 6-1 2D Assembly Power Results

Table 6-2 Pin Power Results

| | Power | Pin Location | Level | Assembly |
|------------|--------|--------------|-------|-----------|
| 2D min rod | 0.1544 | (4,5) | -- | C-14/B-13 |
| 2D max rod | 1.3981 | (17,17) | -- | D-12 |
| 3D min | 0.0246 | (4,5) | 1 | C-14/B-13 |
| 3D max | 1.9756 | (17,17) | 20 | D-12 |

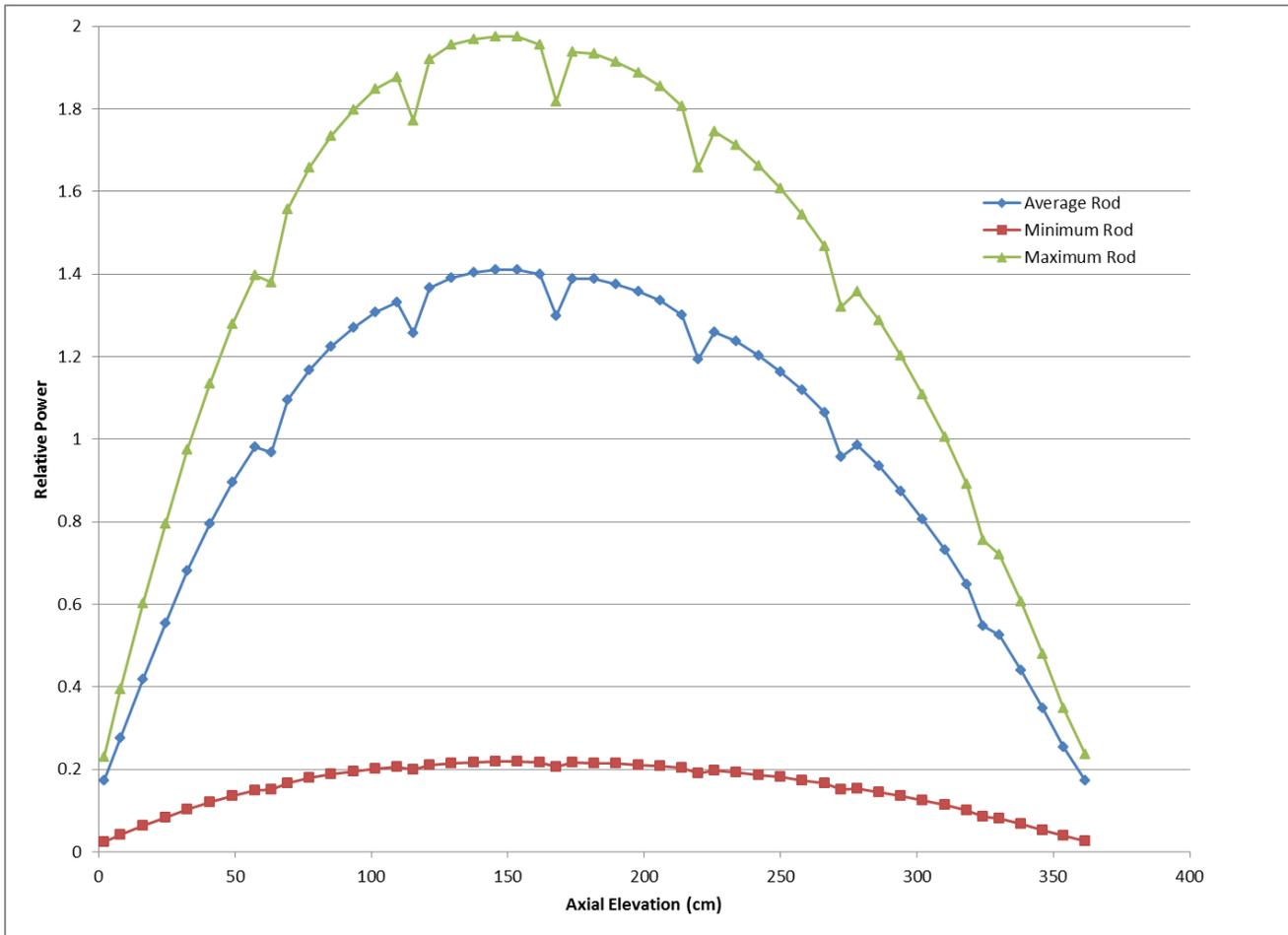


Figure 6-2 Axial Plots of Maximum, Minimum, and Average Rod Powers

Figure 6-3 shows the 3D thermal flux distribution for this problem. The top of the core has been cut off to show the flux distribution in the fuel. The thermal flux is defined as the flux below 0.625 eV. Since most fissions occur at thermal energies, the thermal flux is closely related to the power. Note that the assemblies with Pyrex absorber rods have a lower thermal flux (and power). The thermal flux is also suppressed around the axial grid spacers.

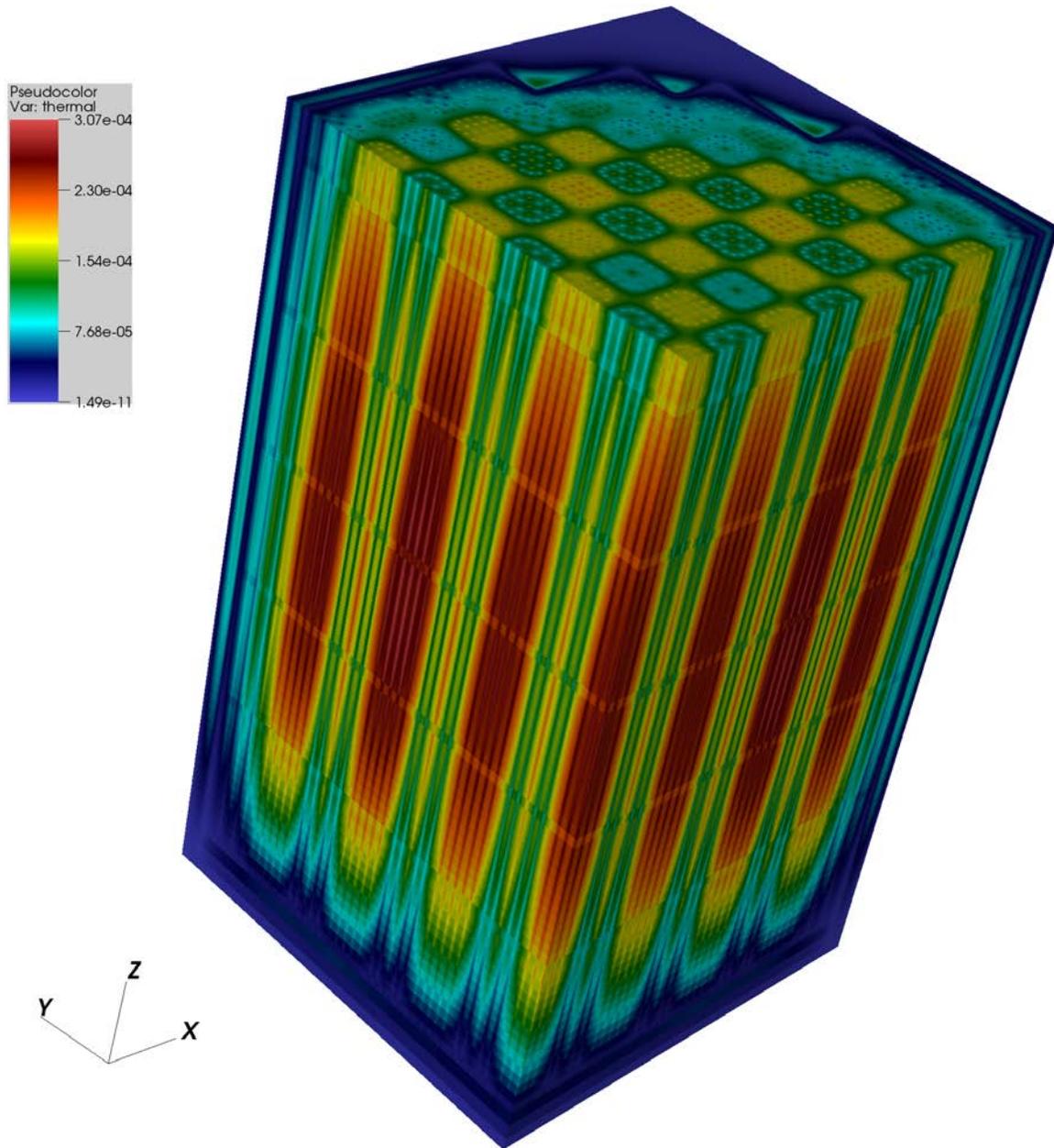


Figure 6-3 3D Thermal Flux Distribution with a cutout at the top of the core

Figure 6-4 shows a 2D slice of the thermal flux near the core midplane. In this figure you can make out where the Pyrex rods are located and you can also see the thermal flux “wings” in the radial reflector region.

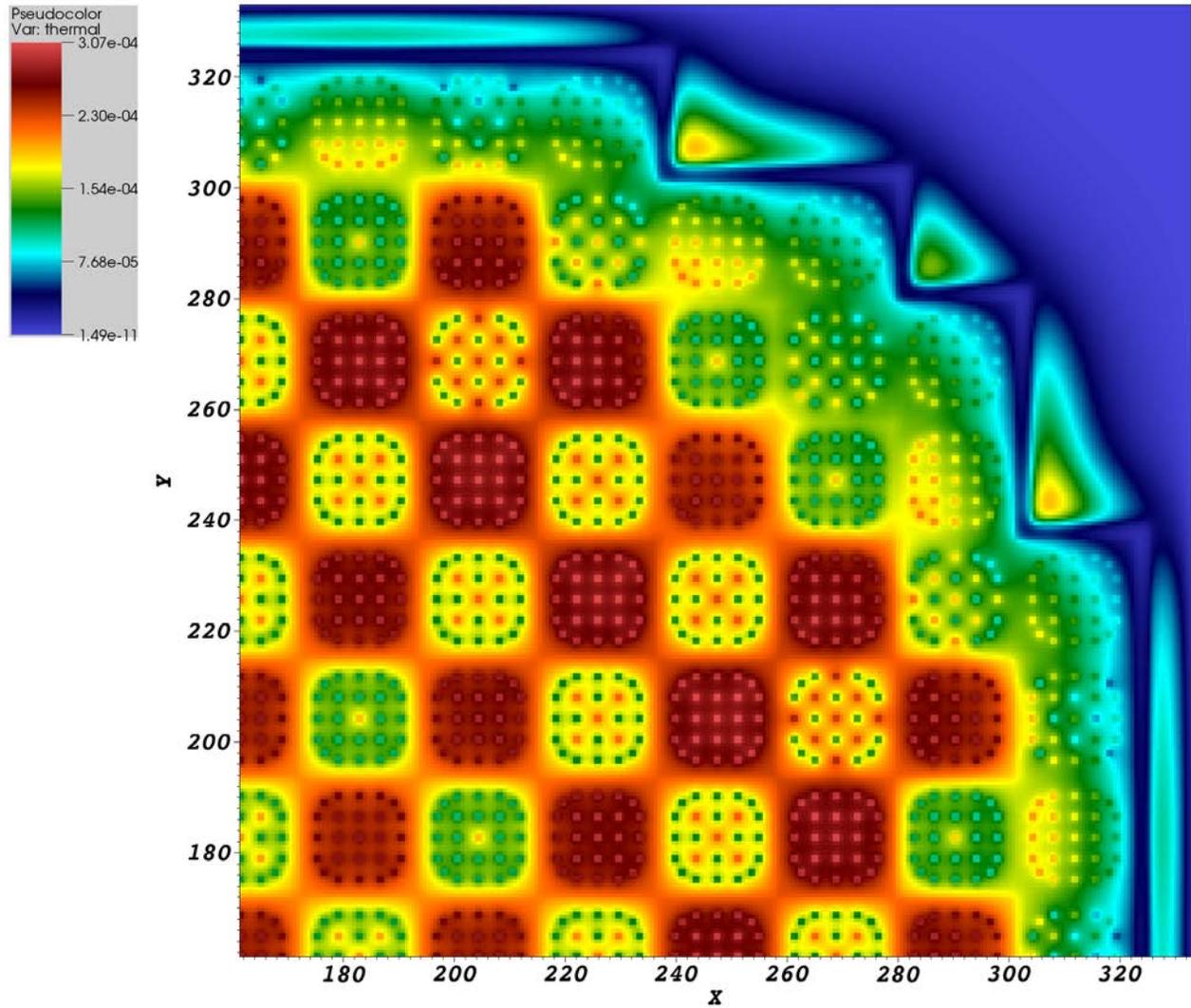


Figure 6-4 2D Slice of Thermal Flux Distribution near the Core Midplane

Figure 6-5 shows a 3D figure of the coolant enthalpy in the active fuel region. This figure shows that the enthalpy rise is not uniform and is closely related to the assembly powers.

Figure 6-6 shows a 2D figure of the coolant enthalpy at the core exit. Note the large enthalpy gradients at the core periphery.

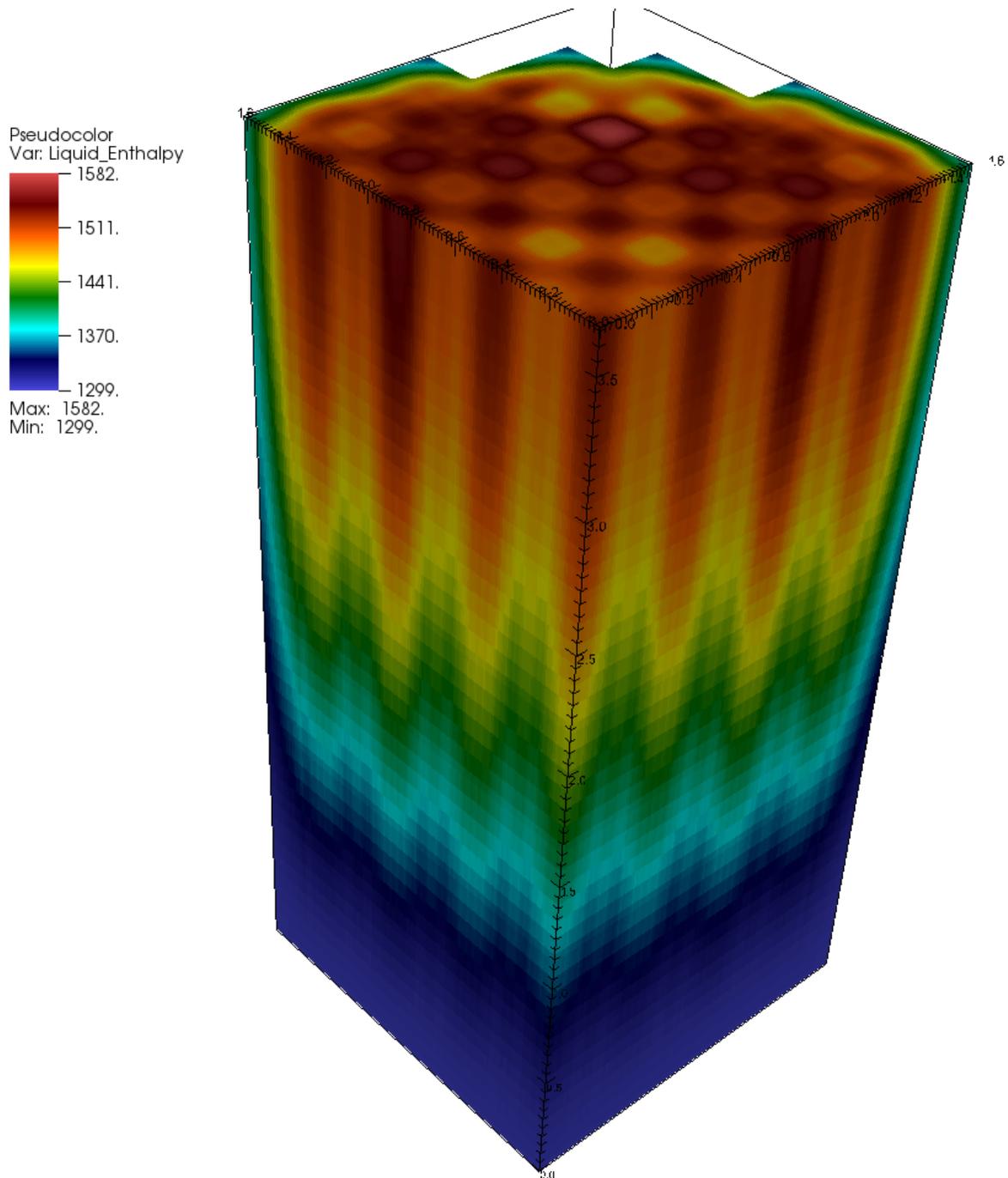


Figure 6-5 3D Coolant Enthalpy Distribution in the active fuel region

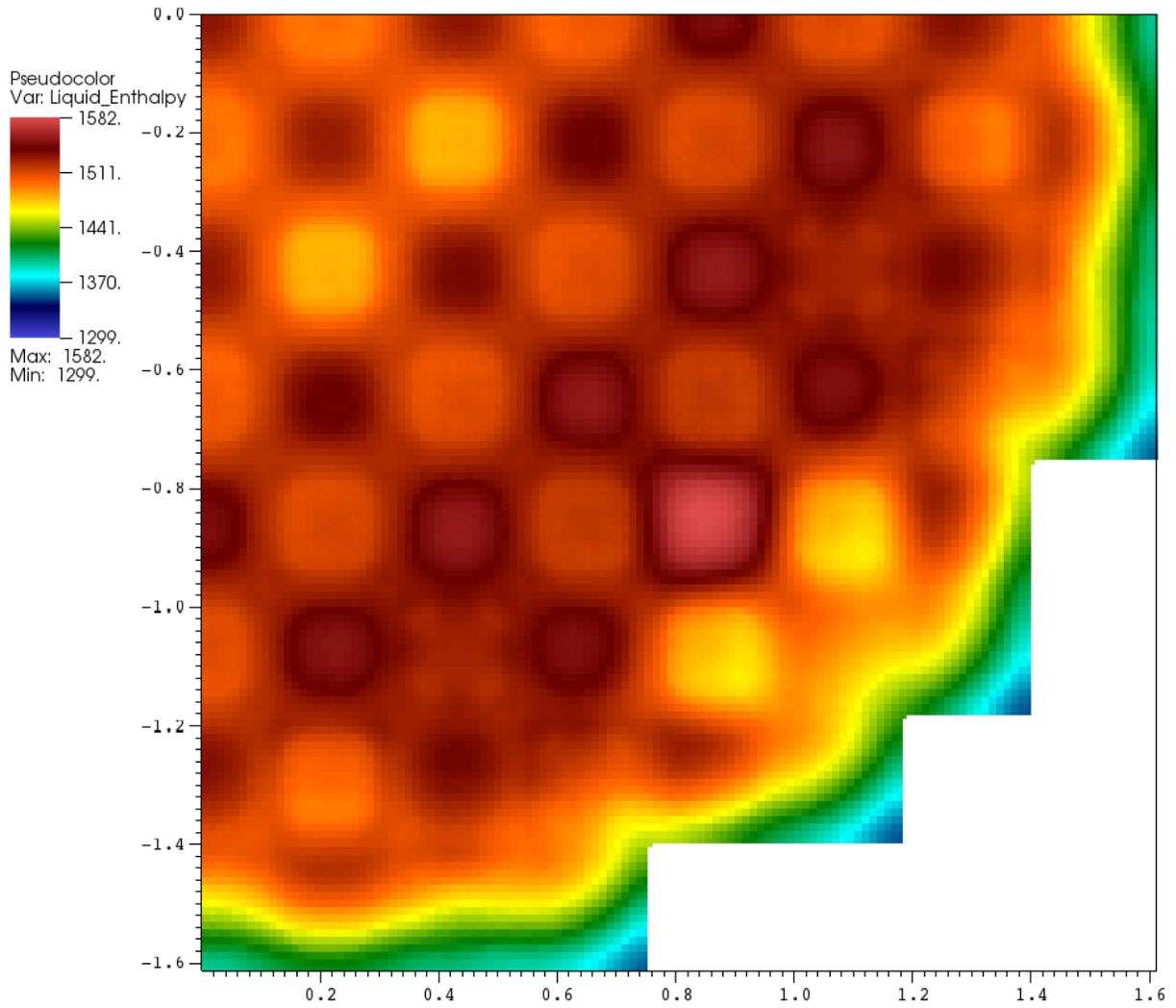


Figure 6-6 Coolant Enthalpy Distribution at the Core Exit

7. Conclusion and Recommendations

This Milestone demonstrates the successful multiphysics coupling of the Insilico neutronics code to the CTF thermal-hydraulics code for a full-core operating reactor. Multiphysics results are shown for several single-assembly cases to demonstrate that the multiphysics coupling is working, and for a full-core operating reactor based on Watts Bar Unit 1 Cycle 1.

This milestone delivers important capability to CASL which includes the ability to model full-core reactors at HZP conditions with:

- 3-D pin-by-pin neutron transport (pin homogenized),
- Multigroup cross sections generated for each unique pincell region with local densities and temperatures,
- 3D subchannel T/H calculations for each rod subchannel in the core, and
- 3D pin-by-pin fuel temperature distributions.

This capability is a significant advance over current industry “nodal methods” which typically have a neutronics, cross section, and T/H resolution of a quarter-assembly.

Future milestones are planned to extend this capability to pin-resolved neutron transport and depletion.

7.1 Recommendations

While this Milestone successfully meets all the objectives of coupling multiphysics codes together, there are still some areas that need to be studied further and/or improved upon. The following further work and improvements are recommended:

1. A convergence study needs to be performed on the Insilico SP_N solver to determine what the recommended code options should be. This includes values for radial mesh, axial mesh, SP_N order, energy group structure, scattering order, and convergence criteria. The effects on run-time should be evaluated along with the recommended code options.
2. A convergence study needs to be performed with CTF to determine what the recommended code options should be. This includes values for the number of rings in the fuel rod conduction model and the number of axial mesh.
3. The fuel temperatures predicted by CTF should be compared to the fuel temperatures predicted by the Peregrine fuel performance code. These comparisons will give confidence in whether the fuel rod conduction model and/or material properties are adequate in CTF.
4. The current iteration strategy using in this code coupling should be studied and improved upon. One suggestion is to implement a dynamic convergence criteria for the neutronics solution that changes with iteration number. Current industry nodal codes have found success using dynamic criteria that sets the neutronics convergence at each coupled iteration to 0.01 times the current convergence observed in the coupled solution. These criteria may reduce the number of neutronics iterations needed at the beginning of the calculation.
5. Investigate methods to improve the restart capability and reduce the number of neutronics iterations required at the start of a restarted calculation. Currently the restart capability works by

starting the CTF calculation from a previously power distribution, but this could be improved by storing additional data from the neutronics solver.

6. Determine the optimal number of cores to run problems on. For example, should users use one core per fuel rod, 4 cores per fuel rod, or something else? The recommendation will probably depend on the library group structure and the number of energy groups used in the 3D transport solver.
7. The current coupling is only using rod-averaged values at each axial elevation. Additional work should be performed to extend this to intra-rod distributions.

8. References

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Appendix A – Property Averaging

This appendix describes how to compute average values in CTF for transfer to Insilico.

A.1 Average coolant properties

Insilico requires an average coolant density and average coolant temperature for each rod. Thus before values can be passed to Insilico, a weighted average of the four surrounding subchannel values must be calculated. These average values are computed in the avg_rod_props subroutine in CTF.

Figure A-1 illustrates how each rod within a PWR assembly is surrounded by four subchannels.

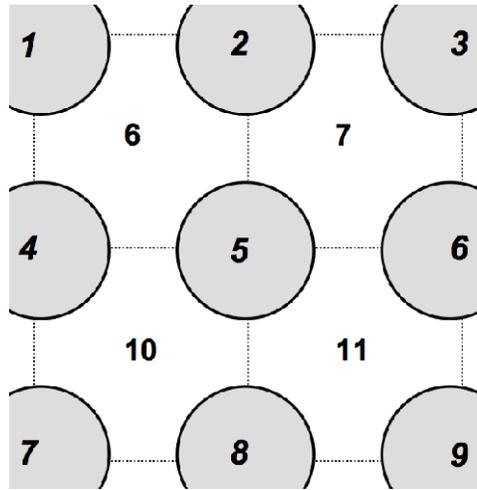


Figure A-1 Illustration of how a typical fuel rod is surrounded by four subchannels in a PWR square lattice fuel assembly.

The average coolant density surrounding fuel rod “n” at axial level “j” is calculated as an area-weighted average of the liquid and vapor densities in the surrounding subchannels (i=1,4) per the following equation.

$$\bar{\rho}_n = \sum_{i=1}^4 \omega_i [(1 - \alpha_i)\rho_{liq(i,j)} + \alpha_i \rho_{vap(i,j)}] \quad (1)$$

where α_i is the volume fraction of the vapor phase, and the normalized weighting factor ω_i is defined in terms of the four surrounding cross sectional areas A_i as

$$\omega_i = \frac{A_i}{\sum_{i=1}^4 A_j} \quad (2)$$

The average coolant temperature surrounding fuel rod “n” at axial level “j” is calculated as a mass-weighted average of the liquid phase temperatures in the surrounding subchannels (i=1,4) per the following equation.

$$\bar{T}_{n,j} = \sum_{i=1}^4 \psi_i T_{i,j} \quad (3)$$

where the normalized mass-weighting factor Ψ_i is defined in terms of the mass of liquid in the four surrounding subchannels (i=1,4)

$$\Psi_i = \frac{A_i \rho_{liq,i}}{\sum_{j=1}^4 A_j \rho_{liq,j}} \quad (4)$$

Note that the vapor-phase contribution is currently neglected because of the very large density difference between vapor and liquid and because of the relative insensitivity of cross sections to small changes in T .

A.2 Average fuel rod properties

Insilico requires an average fuel temperature and average clad temperature for each rod at each axial level. These values must be computed (in the avg_rod_props subroutine) in CTF before they can be passed to Insilico.

CTF resolves the radial variation of temperature within a fuel rod using a finite difference grid as illustrated in Figure A-2. The number of nodes is problem dependent and defined by the user. In Figure A-2 there are five internal nodes together with the requisite fuel pellet surface node and the inner and outer cladding surface nodes (for a total of eight). CTF also has the option to model azimuthal variations with a coarse azimuthal grid that corresponds to the number of subchannels that surround the fuel rod (four in a square lattice).

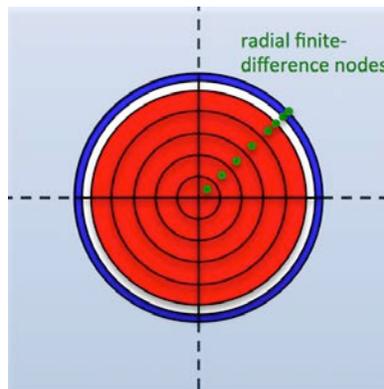


Figure A-2 Illustrative radial discretization of a fuel rod modeled by CTF

The average fuel temperature of fuel rod “n” at axial level “j” is calculated as an area-weighted average of the conduction node temperatures computed by the finite difference heat transfer solution within the fuel rod. This can be expressed as

$$\bar{T}_{f(n,j)} = \sum_{i=1}^{ic-2} \left(\frac{Ar_i}{Af_n} \right) \left[\frac{1}{kla} \sum_{k=1}^{kla} T_{i,n,j,k} \right] \quad (5)$$

where

Ar_i denotes the cross sectional area of radial finite difference node i,

Af_n denotes the total cross sectional area of the fuel,

kla denotes the number of azimuthal sections being modeled, and

ic denotes the total number of radial nodes in the fuel rod heat transfer model (the last 2 rings always refer to the clad material).

The average clad temperature of fuel rod “n” at axial level “j” is calculated in a similar fashion:

$$\bar{T}_{c(n,j)} = \sum_{i=ic-1}^{ic} \left(\frac{Ar_i}{Ac_n} \right) \left[\frac{1}{kla} \sum_{k=1}^{kla} T_{i,n,j,k} \right] \quad (6)$$

where

Ac_n denotes the total cross sectional area of the clad,

and all other terms are as previously defined above.

Appendix B – Single-Assembly Input File

This appendix contains the input listing for a PWR assembly. All of the input for CTF, Insilico, and the coupled code is created through the VERA Common Input.

Input Listing

```
[CASEID]
  title 'CASL Problem 6a'
!=====
! Sample input for Problem 6 (Single-assembly with T/H feedback)
!=====

[STATE]
  power 100.0      ! %
  tinlet 559.0     ! F
  boron 600        ! ppmB
  pressure 2250    ! psia

  tfuel 900.0      ! K - 600K Not used with T/H feedback! set to 900K with feedback
  modden 0.743     ! g/cc Not used with T/H feedback!

  feedback on
  sym full

[CORE]
  size 1           ! 1x1 single-assembly
  rated 17.67 0.6824 ! MW, Mlbs/hr
  apitch 21.50
  height 406.328

  core_shape
  1

  assm_map
  A1

  lower_plate ss 5.0 0.5 ! mat, thickness, vol frac
  upper_plate ss 7.6 0.5 ! mat, thickness, vol frac
  lower_ref mod 26.0 1.0
  upper_ref mod 25.0 1.0

  bc_rad reflecting

  mat he 0.000176
  mat inc 8.19
  mat ss 8.0
  mat zirc 6.56
  mat aic 10.20
  mat pyrex 2.23
  mat b4c 6.56
```

[ASSEMBLY]

title "Westinghouse 17x17"
npin 17
ppitch 1.260

fuel U31 10.257 95.0 / 3.1

| | | | | | | | |
|----------|--------|-------|-------|-------|----|------|-------------------|
| cell 1 | 0.4096 | 0.418 | 0.475 | / U31 | he | zirc | |
| cell 100 | | 0.561 | 0.602 | / mod | | zirc | ! guide tube |
| cell 200 | | 0.561 | 0.602 | / mod | | zirc | ! instrument tube |
| cell 7 | | 0.418 | 0.475 | / mod | | mod | ! empty location |
| cell 8 | | 0.418 | 0.475 | / | he | zirc | ! plenum |
| cell 9 | | | 0.475 | / | | zirc | ! pincap |

lattice FUEL1
200
1 1
1 1 1
100 1 1 100
1 1 1 1 1
1 1 1 1 1 100
100 1 1 100 1 1 1
1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1

lattice LGAP1
200
7 7
7 7 7
100 7 7 100
7 7 7 7 7
7 7 7 7 7 100
100 7 7 100 7 7 7
7 7 7 7 7 7 7 7
7 7 7 7 7 7 7 7 7

lattice PLEN1
200
8 8
8 8 8
100 8 8 100
8 8 8 8 8
8 8 8 8 8 100
100 8 8 100 8 8 8
8 8 8 8 8 8 8 8
8 8 8 8 8 8 8 8 8

lattice PCAP1
200
9 9
9 9 9
100 9 9 100
9 9 9 9 9
9 9 9 9 9 100
100 9 9 100 9 9 9
9 9 9 9 9 9 9 9
9 9 9 9 9 9 9 9 9

axial A1 6.050
LGAP1 10.281
PCAP1 11.951
FUEL1 377.711
PLEN1 393.711
PCAP1 395.381
LGAP1 397.501

```
grid END inc 1017 3.866
grid MID zirc 875 3.810
```

```
grid_axial
  END 13.884
  MID 75.2
  MID 127.4
  MID 179.6
  MID 231.8
  MID 284.0
  MID 336.2
  END 388.2
```

```
lower_nozzle ss 6.05 6250.0 ! mat, height, mass (g)
upper_nozzle ss 8.827 6250.0 ! mat, height, mass (g)
```

[EDITS]

! approximately 3in intervals in active fuel

```
axial_edit_bounds
  11.951
  15.817
  24.028
  32.239
  40.45
  48.662
  56.873
  65.084
  73.295
  77.105
  85.17
  93.235
  101.3
  109.365
  117.43
  125.495
  129.305
  137.37
  145.435
  153.5
  161.565
  169.63
  177.695
  181.505
  189.57
  197.635
  205.7
  213.765
  221.83
  229.895
  233.705
  241.77
  249.835
  257.9
  265.965
  274.03
  282.095
  285.905
  293.97
  302.035
  310.1
  318.165
  326.23
  334.295
```

338.105
346.0262
353.9474
361.8686
369.7898
377.711

[INSILICO]

mat_library casl_comp.sh5
xs_library lib252_hetbondoneabs-noabssigp

max_delta_z 2.54
num_blocks_i 17
num_blocks_j 17
num_z_blocks 12
num_groups 23
num_sets 4
pin_partitioning true

mesh 4
dimension 3
eq_set sc
eigen_solver arnoldi
tolerance 1e-6
Pn_order 0

! eigenvalue_db:
k_tolerance 1e-5
L2_tolerance 1e-5
energy_dep_ev true

! quadrature_db:
quad_type qr
azimuthals_octant 4
polars_octant 4

! silo_db:
silo_output p6
! silo_out_power true

! upscatter_db:
upscatter_tolerance 1e-5

new_grp_bounds
8.2085e+05
1.1109e+05
5.5308e+03
1.8644e+02
3.7612e+01
3.5379e+01
2.7697e+01
2.1684e+01
2.0397e+01
1.5968e+01
7.1500e+00
6.7000e+00
6.3000e+00
1.0970e+00
1.0450e+00
9.5000e-01
3.5000e-01
2.0600e-01
1.0700e-01
5.8000e-02
2.5000e-02

1.0000e-02
1.0000e-05

[COBRATF]

```
nfuel  3          ! number of fuel rings in conduction model
nc      1          ! conduction option - radial conduction
irfc    2          ! friction factor correlation default=2
dhfrac  0.02       ! fraction of power deposited directly into coolant
hgap    5678.3     ! gap conductance
eps0    0.001
oitmax  5
iitmax  40
gridloss END 0.9070 ! spacer grid loss coefficient
gridloss MID 0.9065 ! spacer grid loss coefficient
dtmin   0.000001
dtmax   0.1
tend    0.1
rtwfp   1000.0
maxits  10000
courant 0.8
```

[COUPLING]

```
epsk    5.0 ! pcm
rlx_power 0.5 ! power relaxation factor between coupled iterations
rlx_tfuel 1.0 ! fuel temperature relaxation factor
rlx_den   1.0 ! coolant density relaxation factor
maxiter  100
```

Appendix C – Full-Core Input File

This appendix contains a partial listing for a full-core PWR. All of the input for CTF, Insilico, and the coupled code is created through the VERA Common Input.

Input Listing

```
!  
! Sample Test case for Problem 7 (Full-Core HFP)  
!  
[CASEID]  
  title 'CASL AMA Problem 7 - Watts Bar Unit 1 Cycle 1 - Public'  
  
[STATE]  
  power 100.0           ! %  
  pressure 2250.0  
  feedback on  
  
  tinlet 557.33        ! F - 565K  
  tfuel 900.0          ! K      (HFP value)  
  boron 1285           ! ppmB  
  modden 0.743         ! g/cc  
  sym qtr      ! ***  
  
[CORE]  
  size 15              ! assemblies across core  
  rated 3411 131.68    ! MW, Mlbs/hr  
  apitch 21.5  
  height 406.337  
  
  core_shape  
    0 0 0 0 1 1 1 1 1 1 1 1 0 0 0 0  
    0 0 1 1 1 1 1 1 1 1 1 1 1 1 0 0  
    0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0  
    0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0  
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1  
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1  
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1  
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1  
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1  
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1  
    1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1  
    0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0  
    0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0  
    0 0 1 1 1 1 1 1 1 1 1 1 1 1 0 0  
    0 0 0 0 1 1 1 1 1 1 1 1 0 0 0 0  
  
  assm_map  
    1  
    2 1  
    1 2 1  
    2 1 2 1  
    1 2 1 2 2  
    2 1 2 1 2 3  
    1 3 1 3 3 3  
    3 3 3 3
```

```

insert_map
-
20 -
- 24 -
20 - 20 -
- 20 - 20 -
20 - 16 - 24 12
- 24 - 16 - -
12 - 8 -

baffle ss 0.19 2.85      ! material, gap, baffle thickness
vessel mod 219.71 cs 241.70 ! material, radii, material, radii

lower_plate ss 5.0 0.5  ! mat, thickness, vol frac
upper_plate ss 7.6 0.5  ! mat, thickness, vol frac

xlabel R P N M L K J H G F E D C B A
ylabel 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

mat he      0.0001786
mat inc     8.19
mat ss      8.0
mat zirc    6.56 zirc4

```

[ASSEMBLY]

[INSERT]

[CONTROL]

[EDITS]

[INSILICO]

[COBRATF]

[COUPLING]